Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH +)   1.02   ±0.07 (n=50)
logP (neutral X)   3.79   ±0.02 (n=50)

18C-01012 Points 1 to 21

M12_octanol concentration factor   0.790
Carbonate   0.0885 mM
Acidity error   -0.75786 mM

18C-01012 Points 22 to 45

M12_octanol concentration factor   0.666
Carbonate   0.1221 mM
Acidity error   -0.39695 mM

18C-01012 Points 46 to 87

M12_octanol concentration factor   0.461
Carbonate   1.9011 mM
Acidity error   -0.34659 mM

Warnings and errors

Errors   None
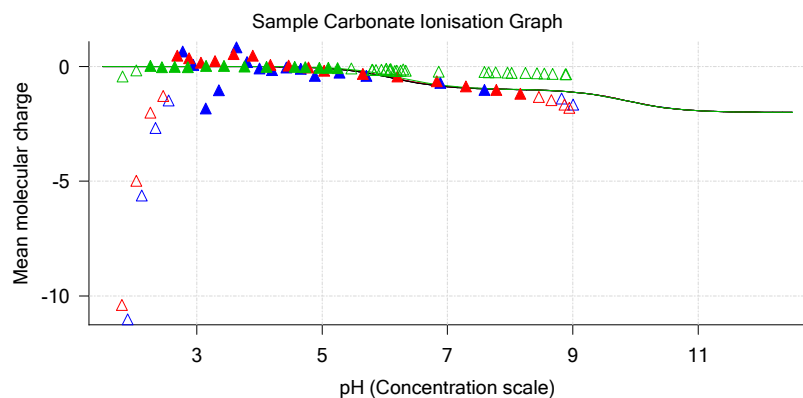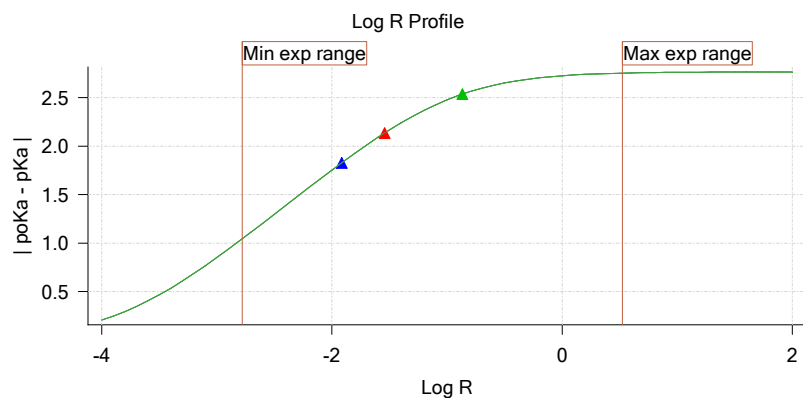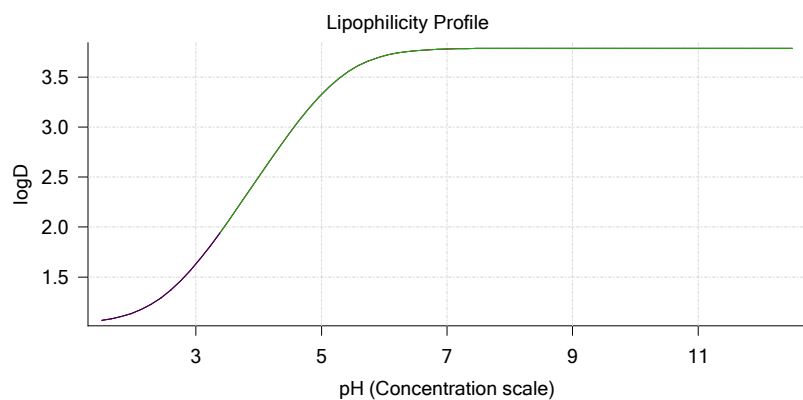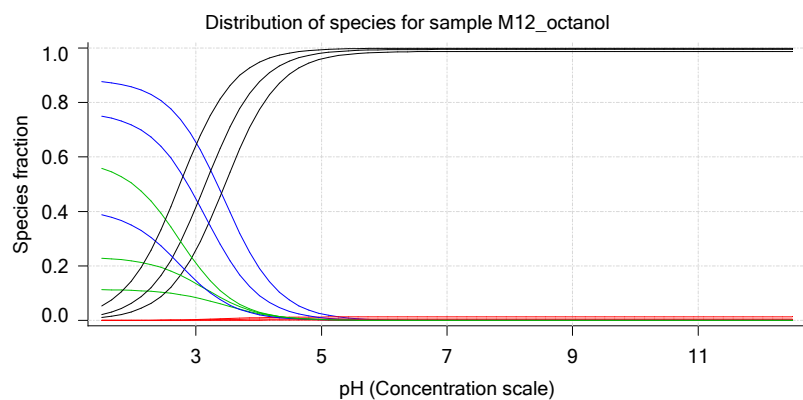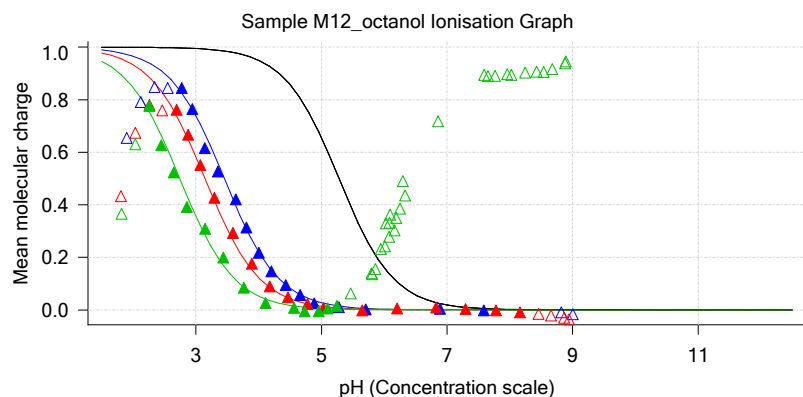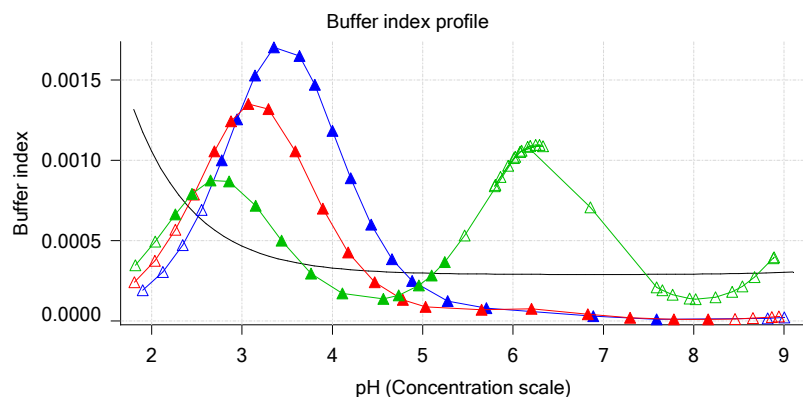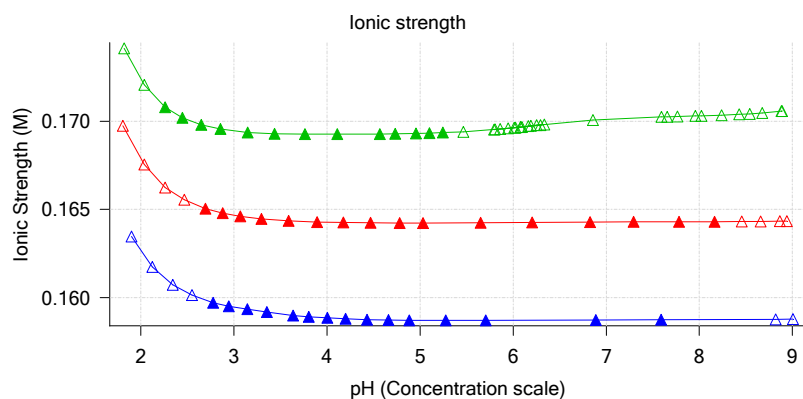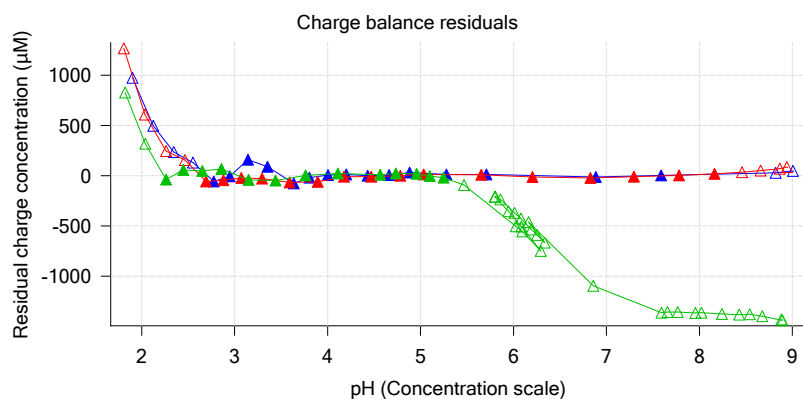Warnings   Excessive carbonate concentration present

Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.04	8.40 %	0.00 %	88.90 %	2.71 %	
1.200	1.05	8.26 %	0.00 %	87.51 %	4.23 %	Stomach pH
2.000	1.14	6.75 %	0.00 %	71.47 %	21.78 %	
3.000	1.63	2.28 %	0.01 %	24.14 %	73.56 %	
4.000	2.50	0.30 %	0.02 %	3.17 %	96.52 %	
5.000	3.33	0.03 %	0.02 %	0.33 %	99.63 %	
6.000	3.71	0.00 %	0.02 %	0.03 %	99.95 %	
6.500	3.76	0.00 %	0.02 %	0.01 %	99.97 %	
7.000	3.78	0.00 %	0.02 %	0.00 %	99.98 %	
7.400	3.79	0.00 %	0.02 %	0.00 %	99.98 %	Blood pH
8.000	3.79	0.00 %	0.02 %	0.00 %	99.98 %	
9.000	3.79	0.00 %	0.02 %	0.00 %	99.98 %	
10.000	3.79	0.00 %	0.02 %	0.00 %	99.98 %	
11.000	3.79	0.00 %	0.02 %	0.00 %	99.98 %	
12.000	3.79	0.00 %	0.02 %	0.00 %	99.98 %	

Sample name: **M12_octanol** Experiment start time: **3/1/2018 3:28:52 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-01012** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M12_octanol Ionisation Graph

Distribution of species for sample M12_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Graphs (continued)

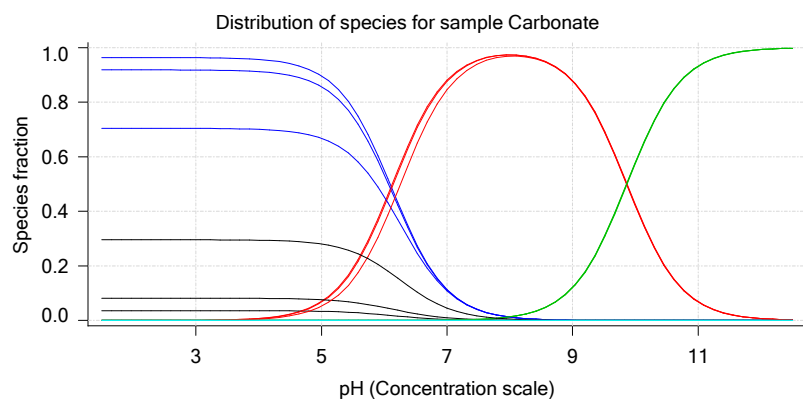Distribution of species for sample Carbonate

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 1 of 3   18C-01012 Points 1 to 21

Overall results

RMSD	0.175
Average ionic strength	0.159 M
Average temperature	25.0°C
Partition ratio	0.0122 : 1
Analyte concentration range	3733.6 µM to 3842.7 µM
Total points considered	15 of 21

Warnings and errors

Errors   None
Warnings   None

Four-Plus parameters

	Alpha	0.130	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
	S	0.9970	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
	jH	0.8	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
	jOH	-0.4	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r

Titrants

	0.50 M HCl	0.993513	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
	0.50 M KOH	0.999845	3/1/2018 3:28:52 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M12_octanol concentration factor	0.790
M12_octanol stoichiometry	1.000
Chloride stoichiometry	1.000
Base pKa 1	5.28
logP (XH +)	1.53
logP (neutral X)	3.90

Sample graphs

Ionisation of sample M12_octanol

Distribution of species for sample M12_octanol

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
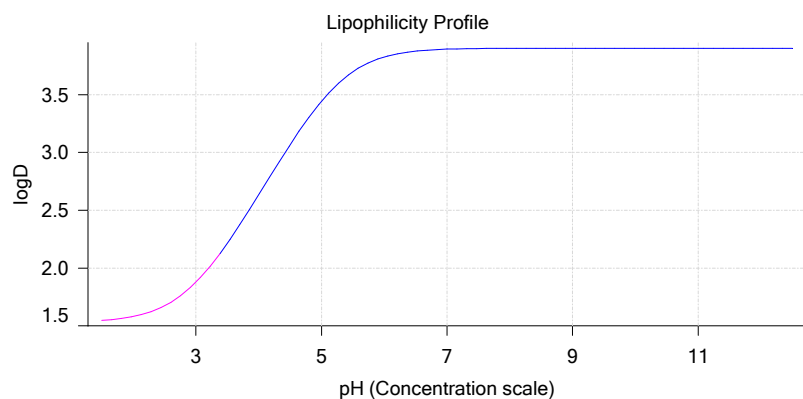
Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.54	70.54 %	0.00 %	29.09 %	0.36 %	
1.200	1.54	70.39 %	0.01 %	29.03 %	0.57 %	Stomach pH
2.000	1.58	68.31 %	0.04 %	28.17 %	3.48 %	
3.000	1.88	51.88 %	0.27 %	21.40 %	26.45 %	
4.000	2.63	15.23 %	0.80 %	6.28 %	77.68 %	
5.000	3.44	1.89 %	0.99 %	0.78 %	96.34 %	
6.000	3.83	0.19 %	1.02 %	0.08 %	98.71 %	
6.500	3.88	0.06 %	1.02 %	0.03 %	98.90 %	
7.000	3.89	0.02 %	1.02 %	0.01 %	98.95 %	
7.400	3.90	0.01 %	1.02 %	0.00 %	98.97 %	Blood pH
8.000	3.90	0.00 %	1.02 %	0.00 %	98.98 %	
9.000	3.90	0.00 %	1.02 %	0.00 %	98.98 %	
10.000	3.90	0.00 %	1.02 %	0.00 %	98.98 %	
11.000	3.90	0.00 %	1.02 %	0.00 %	98.98 %	
12.000	3.90	0.00 %	1.02 %	0.00 %	98.98 %	

Carbonate and acidity

Carbonate 0.088 mM
Acidity error -0.758 mM

Other graphs

Assay progress

Titration graph

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
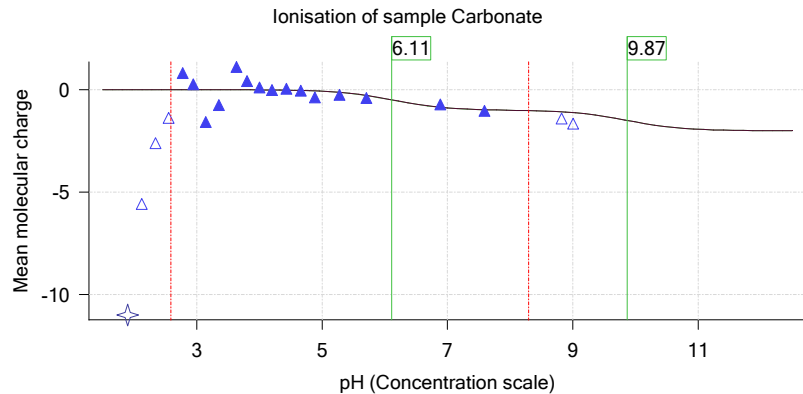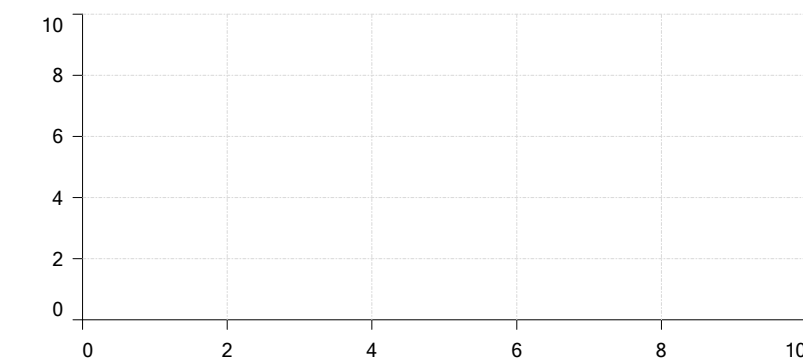
Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 2 of 3   18C-01012 Points 22 to 45

Overall results

RMSD   0.444
Average ionic strength   0.164 M
Average temperature   25.0°C
Partition ratio   0.0288 : 1
Analyte concentration range   3433.0 µM to 3545.2 µM
Total points considered   16 of 24

Warnings and errors

Errors   None
Warnings   Sample concentration factor out of range

Four-Plus parameters

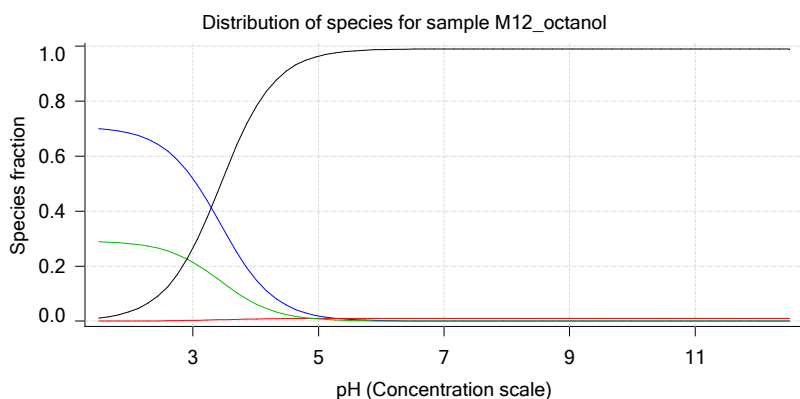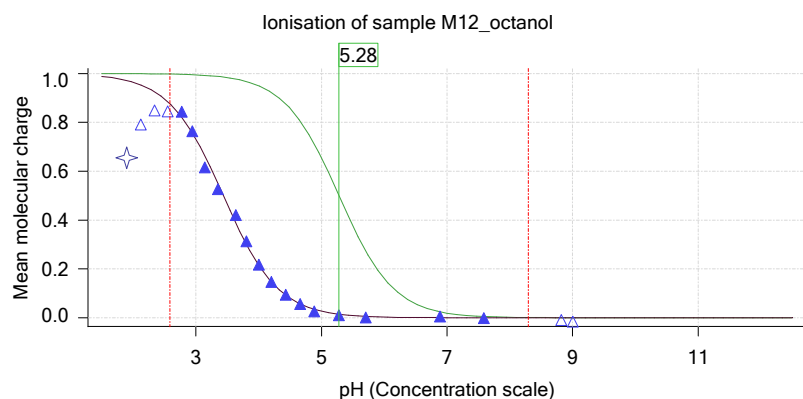|				
🔒	Alpha	0.130	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
🔒	S	0.9970	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
🔒	jH	0.8	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
🔒	jOH	-0.4	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r

Titrants

🔒	0.50 M HCl	0.993513	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
🔒	0.50 M KOH	0.999845	3/1/2018 3:28:52 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

🔷	M12_octanol concentration factor	0.666
🔒	M12_octanol stoichiometry	1.000
🔒	Chloride stoichiometry	1.000
🔒	Base pKa 1	5.28
🔒	logP (XH +)	1.53
🔷	logP (neutral X)	3.93

Sample graphs

Ionisation of sample M12_octanol

Distribution of species for sample M12_octanol

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
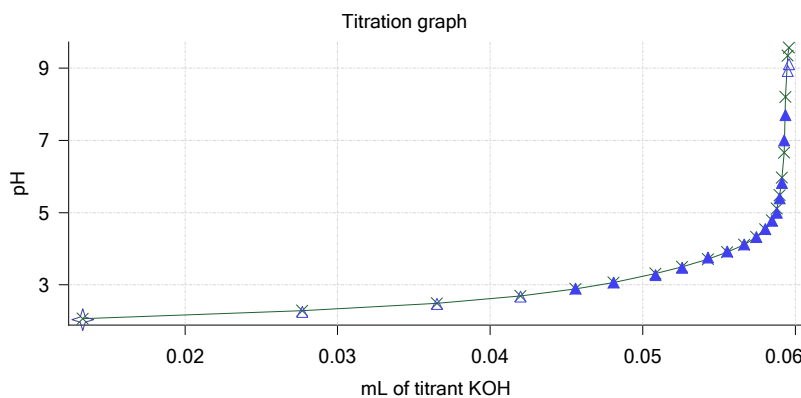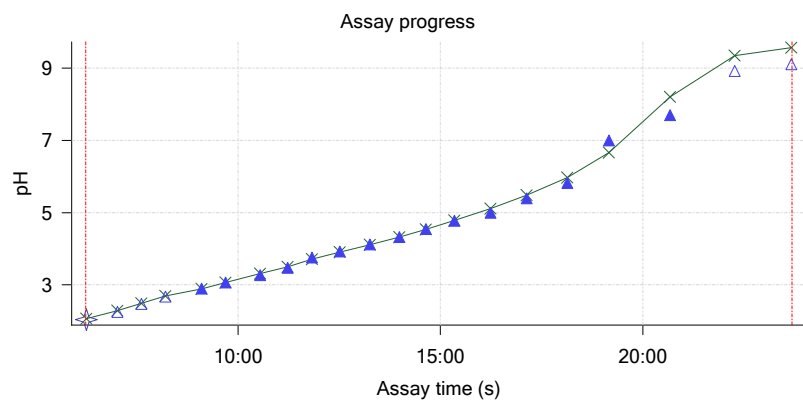Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
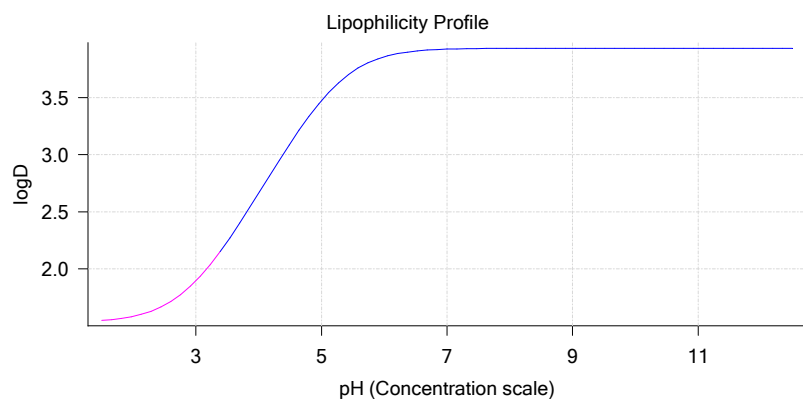
Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.54	50.30 %	0.00 %	49.05 %	0.65 %	
1.200	1.54	50.10 %	0.00 %	48.86 %	1.03 %	Stomach pH
2.000	1.58	47.50 %	0.02 %	46.32 %	6.15 %	
3.000	1.89	30.53 %	0.16 %	29.77 %	39.54 %	
4.000	2.66	6.68 %	0.35 %	6.51 %	86.46 %	
5.000	3.47	0.76 %	0.40 %	0.74 %	98.11 %	
6.000	3.86	0.08 %	0.40 %	0.07 %	99.45 %	
6.500	3.91	0.02 %	0.40 %	0.02 %	99.55 %	
7.000	3.92	0.01 %	0.40 %	0.01 %	99.58 %	
7.400	3.93	0.00 %	0.40 %	0.00 %	99.59 %	Blood pH
8.000	3.93	0.00 %	0.40 %	0.00 %	99.59 %	
9.000	3.93	0.00 %	0.40 %	0.00 %	99.60 %	
10.000	3.93	0.00 %	0.40 %	0.00 %	99.60 %	
11.000	3.93	0.00 %	0.40 %	0.00 %	99.60 %	
12.000	3.93	0.00 %	0.40 %	0.00 %	99.60 %	

Carbonate and acidity

Carbonate 0.122 mM
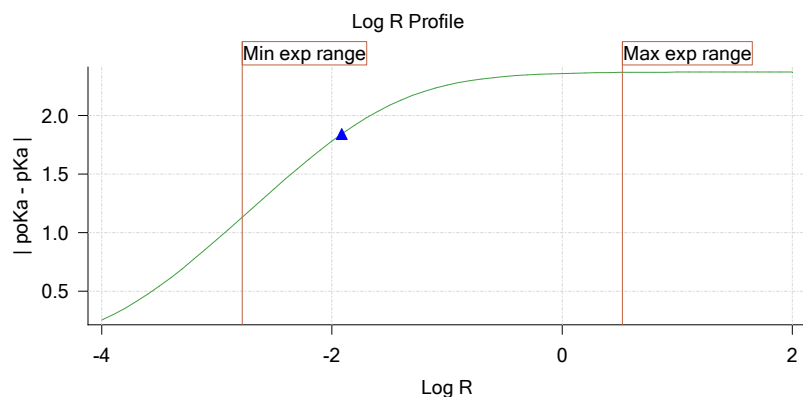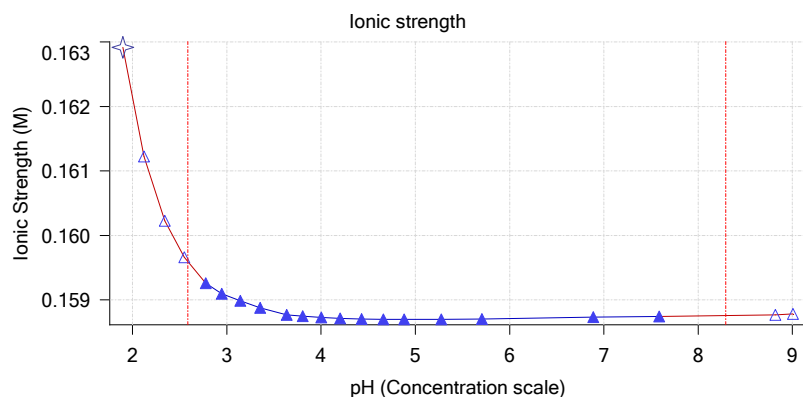Acidity error -0.397 mM

Other graphs

Assay progress

Titration graph
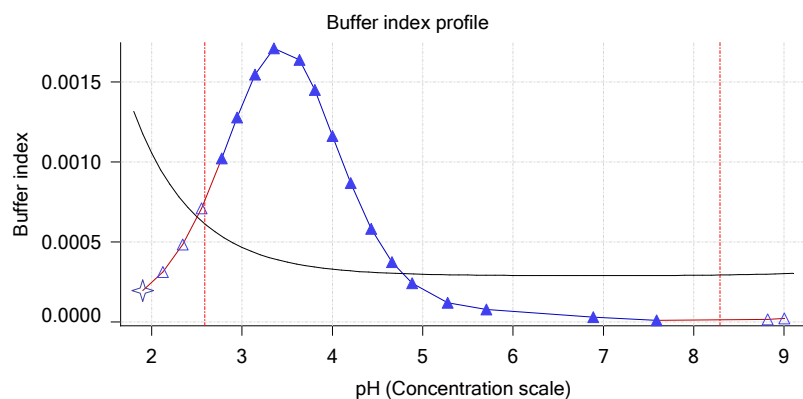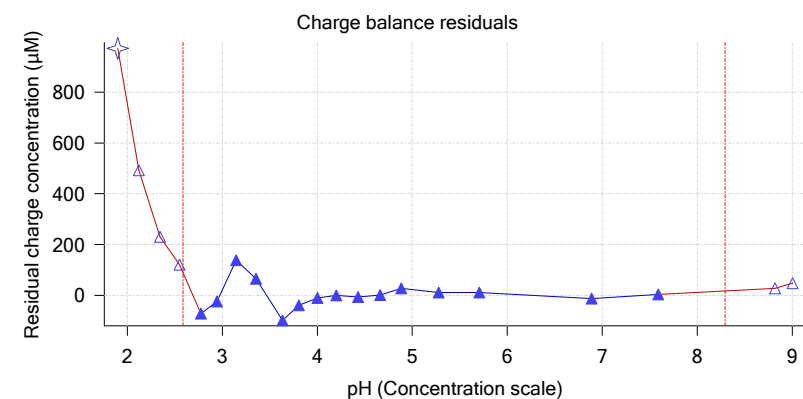
Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
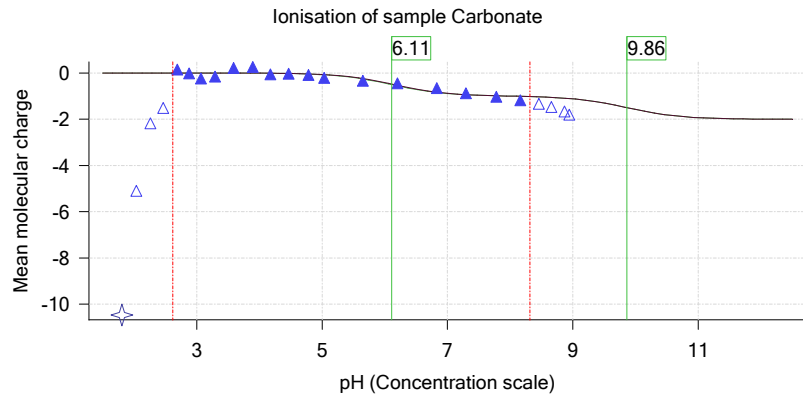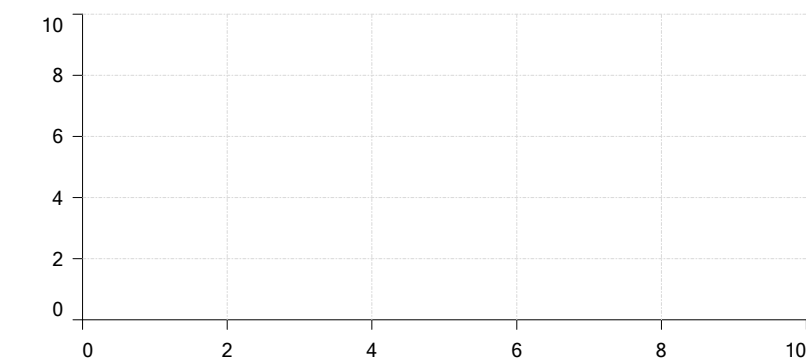
Sample name: **M12_octanol**   Experiment start time: **3/1/2018 3:28:52 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01012**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

pH-metric high logP   Titration 3 of 3   18C-01012 Points 46 to 87

Overall results

RMSD   0.047
Average ionic strength   0.169 M
Average temperature   25.0°C
Partition ratio   0.1359 : 1
Analyte concentration range   2911.0 µM to 2994.8 µM
Total points considered   13 of 42

Warnings and errors

Errors   None
Warnings   Sample concentration factor out of range
            Excessive carbonate concentration present

Four-Plus parameters

Alpha   0.130   3/1/2018 3:28:52 PM   C:\Sirius_T3\HCl18B27.t3r
S   0.9970   3/1/2018 3:28:52 PM   C:\Sirius_T3\HCl18B27.t3r
jH   0.8   3/1/2018 3:28:52 PM   C:\Sirius_T3\HCl18B27.t3r
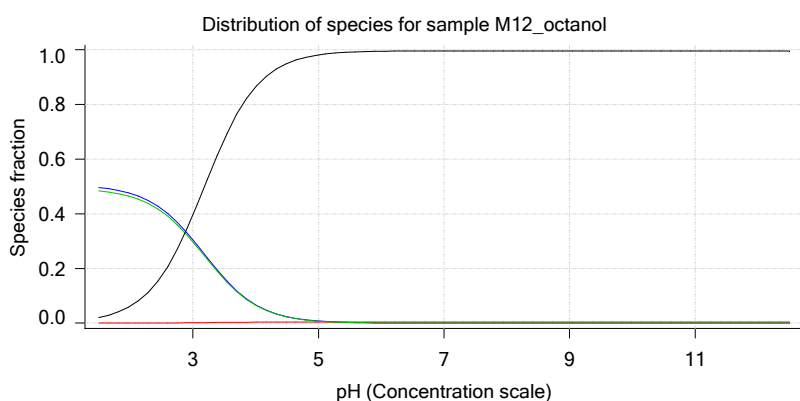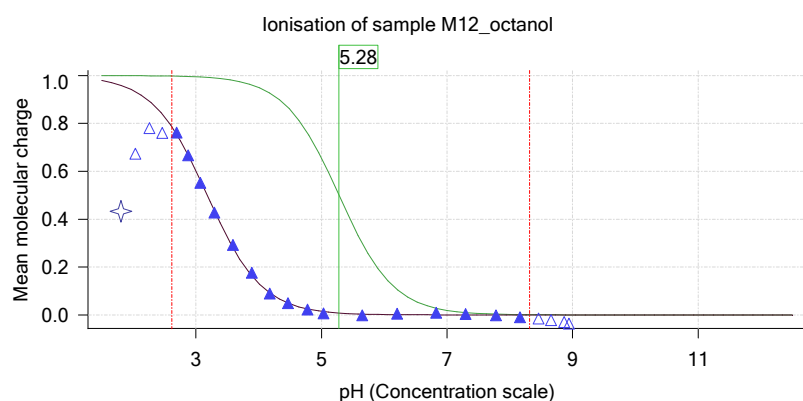jOH   -0.4   3/1/2018 3:28:52 PM   C:\Sirius_T3\HCl18B27.t3r

Titrants

0.50 M HCl   0.993513   3/1/2018 3:28:52 PM   C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH   0.999845   3/1/2018 3:28:52 PM   C:\Sirius_T3\KOH18B27.t3r

Sample

M12_octanol concentration factor   0.461
M12_octanol stoichiometry   1.000
Chloride stoichiometry   1.000
Base pKa 1   5.28
logP (XH +)   1.53
logP (neutral X)   4.17

Sample graphs

Ionisation of sample M12_octanol

Distribution of species for sample M12_octanol

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
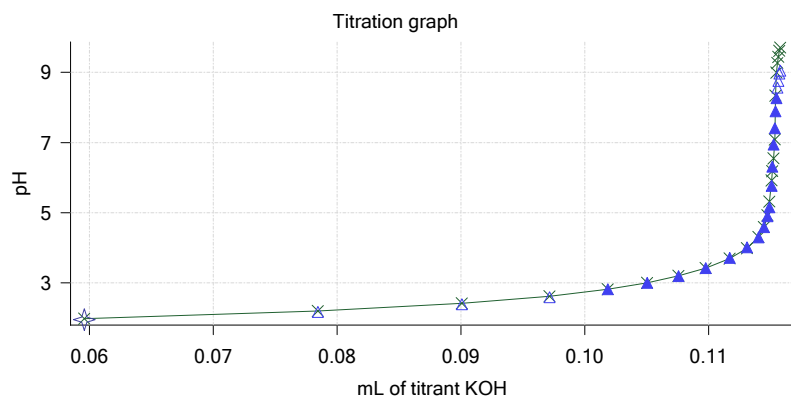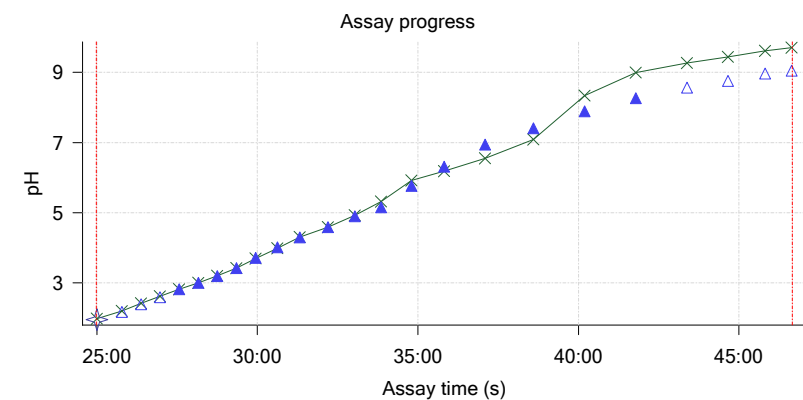Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
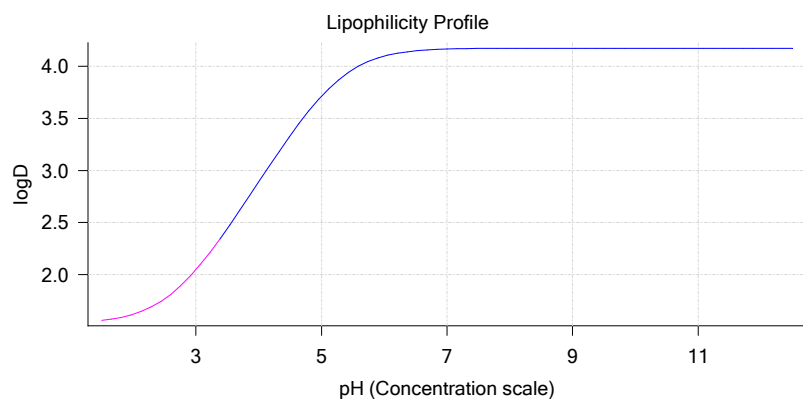
Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.54	17.51 %	0.00 %	80.63 %	1.86 %	
1.200	1.55	17.32 %	0.00 %	79.76 %	2.92 %	Stomach pH
2.000	1.62	15.00 %	0.01 %	69.06 %	15.93 %	
3.000	2.05	6.16 %	0.03 %	28.37 %	65.44 %	
4.000	2.89	0.89 %	0.05 %	4.12 %	94.94 %	
5.000	3.71	0.09 %	0.05 %	0.43 %	99.43 %	
6.000	4.10	0.01 %	0.05 %	0.04 %	99.90 %	
6.500	4.15	0.00 %	0.05 %	0.01 %	99.93 %	
7.000	4.16	0.00 %	0.05 %	0.00 %	99.95 %	
7.400	4.17	0.00 %	0.05 %	0.00 %	99.95 %	Blood pH
8.000	4.17	0.00 %	0.05 %	0.00 %	99.95 %	
9.000	4.17	0.00 %	0.05 %	0.00 %	99.95 %	
10.000	4.17	0.00 %	0.05 %	0.00 %	99.95 %	
11.000	4.17	0.00 %	0.05 %	0.00 %	99.95 %	
12.000	4.17	0.00 %	0.05 %	0.00 %	99.95 %	

Carbonate and acidity

Carbonate   1.901 mM
Acidity error   -0.347 mM

Other graphs
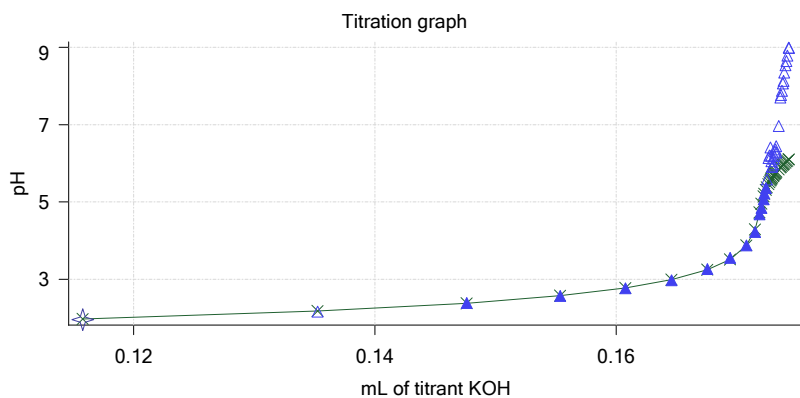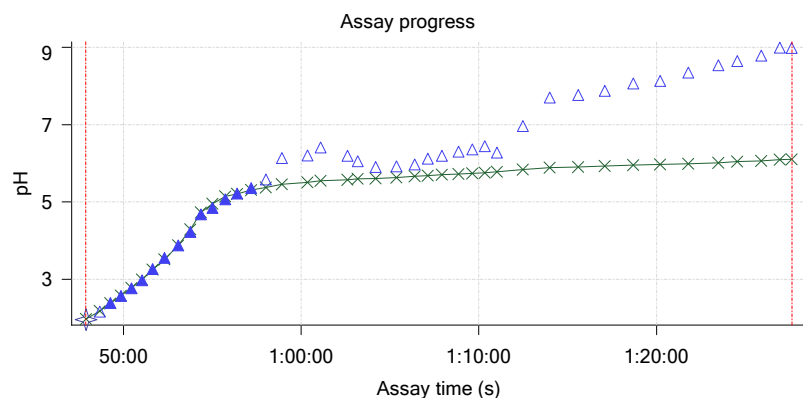
Assay progress

Titration graph

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Min exp range

Max exp range
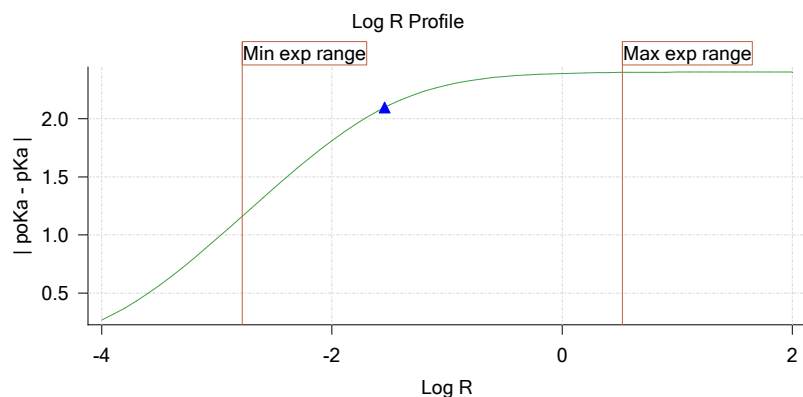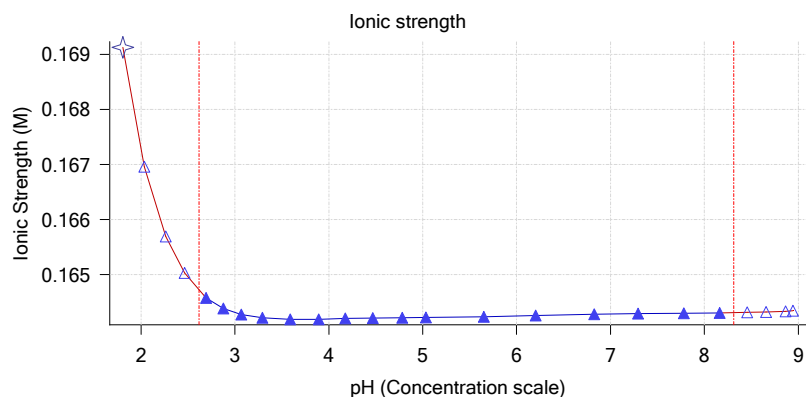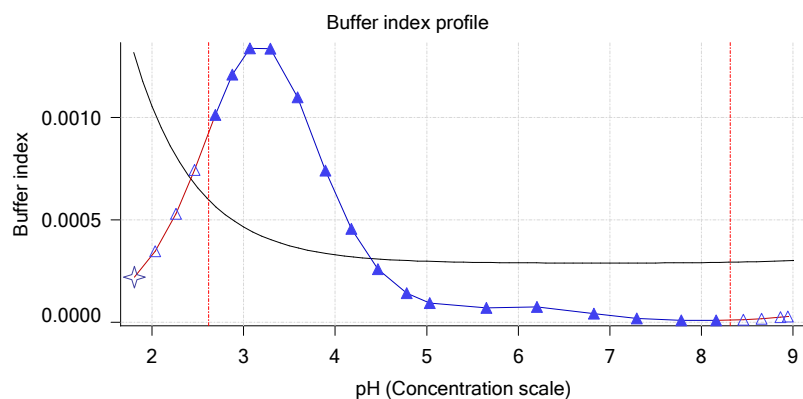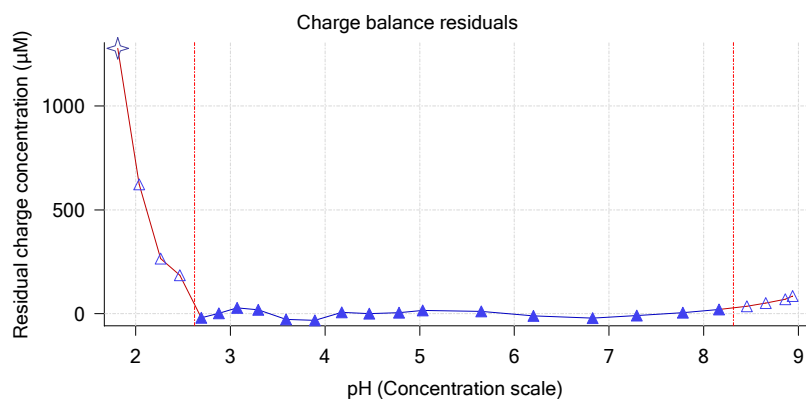
Ionisation of sample Carbonate

6.11

9.86
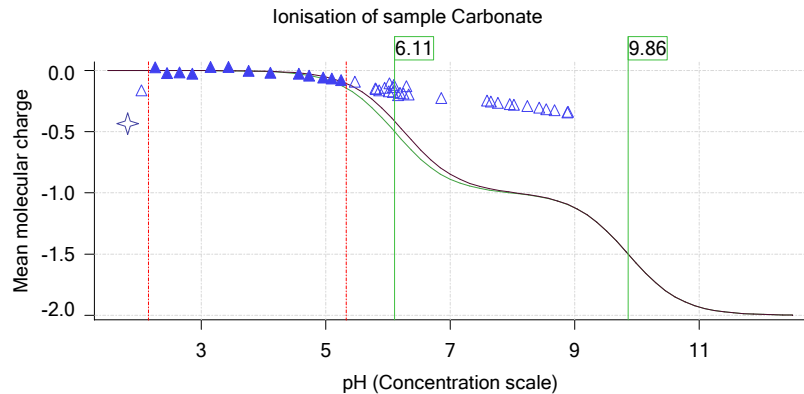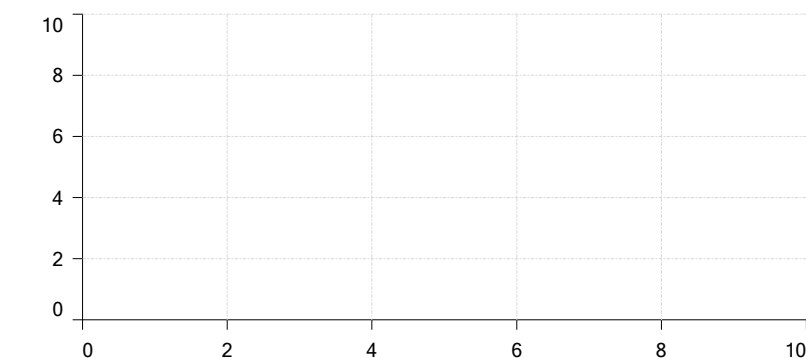
Assay model

Sample name: **M12_octanol**

Assay name: **pH-metric high logP**

Assay ID: **18C-01012**

Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**

Analyst: **Pion**

Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M12_octanol	2/28/2018 2:58:36 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001780 g	2/28/2018 4:51:40 PM	User entered value
Formula weight	292.16 g/mol	2/28/2018 2:58:36 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	255.70	2/28/2018 2:58:36 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/28/2018 2:58:36 PM	User entered value
Sample is a	Base	2/28/2018 2:58:36 PM	User entered value
pKa 1	5.28	2/28/2018 2:58:36 PM	User entered value
logp (XH +)	1.53	2/28/2018 2:59:16 PM	User entered value
logP (neutral X)	3.50	2/28/2018 2:59:06 PM	User entered value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

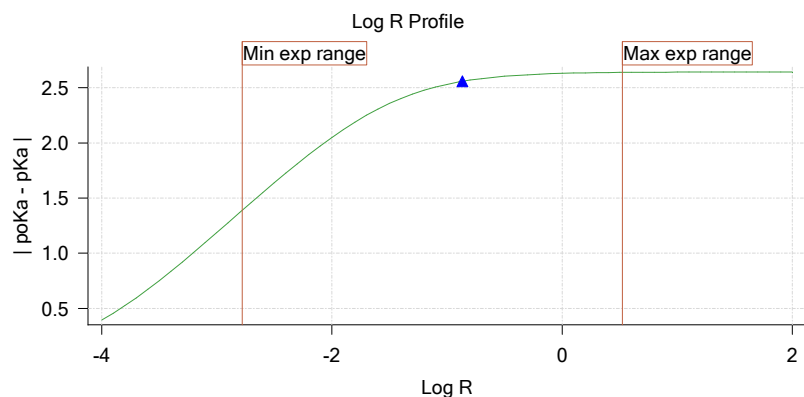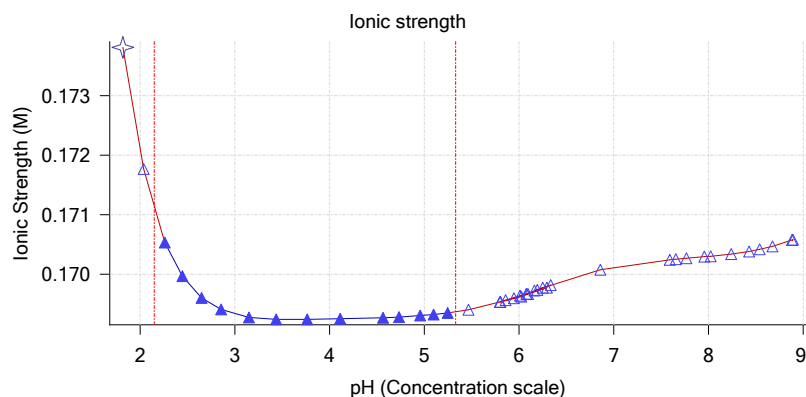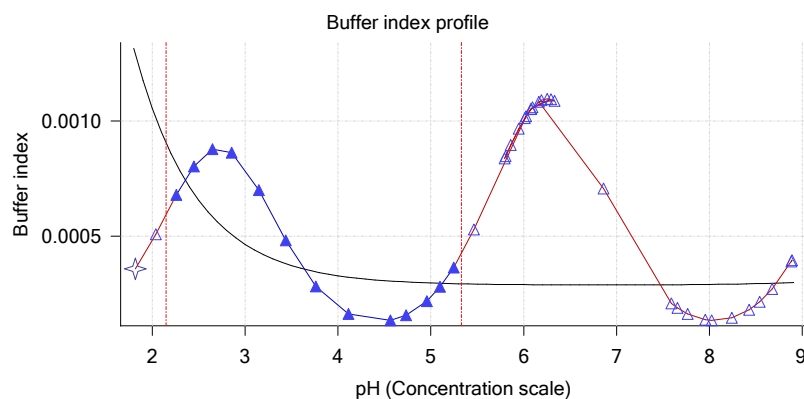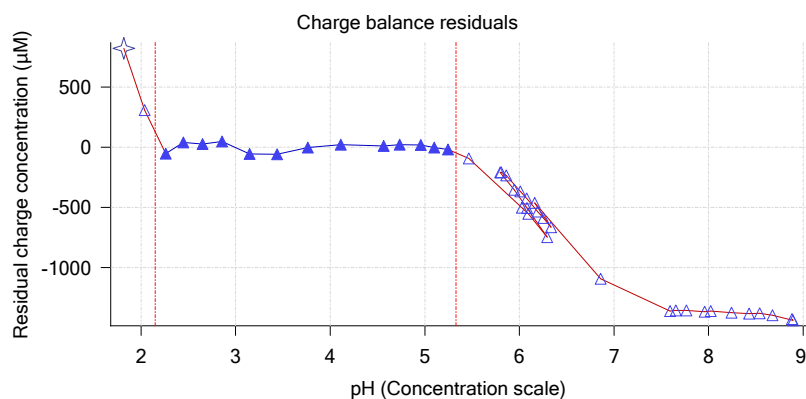| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
3:15.3	Initial pH = 4.96									
6:15.1	Data point 1	1.50000 mL	0.05221 mL	0.01329 mL	0.01999 mL	2.033	-0.00115	0.13540	0.00015	10.0 s
7:01.4	Data point 2	1.50000 mL	0.05221 mL	0.02768 mL	0.01999 mL	2.252	0.00111	0.19272	0.00012	10.0 s
7:37.0	Data point 3	1.50000 mL	0.05221 mL	0.03652 mL	0.01999 mL	2.470	-0.00312	0.03211	0.00086	10.0 s
8:12.5	Data point 4	1.50000 mL	0.05221 mL	0.04198 mL	0.01999 mL	2.675	-0.00299	0.02511	0.00093	28.0 s
9:06.1	Data point 5	1.50000 mL	0.05221 mL	0.04560 mL	0.01999 mL	2.899	0.00724	0.28037	0.00067	10.0 s
9:41.6	Data point 6	1.50000 mL	0.05221 mL	0.04809 mL	0.01999 mL	3.067	-0.00758	0.65584	0.00046	10.0 s
10:32.6	Data point 7	1.50000 mL	0.05221 mL	0.05085 mL	0.01999 mL	3.266	-0.00574	0.79317	0.00032	10.5 s
11:13.7	Data point 8	1.50000 mL	0.05221 mL	0.05259 mL	0.01999 mL	3.474	-0.01919	0.98927	0.00095	10.5 s
11:49.7	Data point 9	1.50000 mL	0.05221 mL	0.05428 mL	0.01999 mL	3.755	-0.01633	0.83230	0.00088	10.5 s
12:30.9	Data point 10	1.50000 mL	0.05221 mL	0.05555 mL	0.01999 mL	3.923	-0.01859	0.95788	0.00094	14.0 s
13:15.5	Data point 11	1.50000 mL	0.05221 mL	0.05666 mL	0.01999 mL	4.120	-0.01675	0.71331	0.00098	13.0 s
13:59.1	Data point 12	1.50000 mL	0.05221 mL	0.05746 mL	0.01999 mL	4.319	-0.01672	0.90369	0.00087	14.0 s
14:38.5	Data point 13	1.50000 mL	0.05221 mL	0.05804 mL	0.01999 mL	4.547	-0.01987	0.96798	0.00100	17.0 s
15:21.0	Data point 14	1.50000 mL	0.05221 mL	0.05847 mL	0.01999 mL	4.777	-0.01763	0.88444	0.00093	23.0 s
16:14.5	Data point 15	1.50000 mL	0.05221 mL	0.05880 mL	0.01999 mL	4.998	-0.01818	0.93024	0.00093	28.0 s
17:08.0	Data point 16	1.50000 mL	0.05221 mL	0.05898 mL	0.01999 mL	5.391	-0.01937	0.94705	0.00098	29.5 s
18:08.0	Data point 17	1.50000 mL	0.05221 mL	0.05913 mL	0.01999 mL	5.819	-0.01888	0.96763	0.00095	31.5 s
19:10.1	Data point 18	1.50000 mL	0.05221 mL	0.05927 mL	0.01999 mL	6.996	-0.07112	0.99199	0.00353	Timed out at 59.5 s
20:40.6	Data point 19	1.50000 mL	0.05221 mL	0.05936 mL	0.01999 mL	7.695	-0.08201	0.99679	0.00406	Timed out at 59.5 s
22:16.3	Data point 20	1.50000 mL	0.05221 mL	0.05950 mL	0.01999 mL	8.922	-0.00844	0.17826	0.00099	53.5 s
23:40.4	Data point 21	1.50000 mL	0.05221 mL	0.05960 mL	0.01999 mL	9.107	-0.02002	0.98651	0.00100	26.0 s
25:00.1	Data point 22	1.50000 mL	0.10891 mL	0.05960 mL	0.05000 mL	1.945	-0.00363	0.51184	0.00025	10.5 s
25:46.8	Data point 23	1.50000 mL	0.10891 mL	0.07846 mL	0.05000 mL	2.167	0.00370	0.60390	0.00024	10.0 s
26:22.5	Data point 24	1.50000 mL	0.10891 mL	0.09008 mL	0.05000 mL	2.390	-0.00263	0.03650	0.00068	10.0 s
26:58.0	Data point 25	1.50000 mL	0.10891 mL	0.09715 mL	0.05000 mL	2.592	0.00780	0.23852	0.00079	10.5 s
27:34.1	Data point 26	1.50000 mL	0.10891 mL	0.10186 mL	0.05000 mL	2.817	0.00513	0.20428	0.00056	10.0 s
28:09.6	Data point 27	1.50000 mL	0.10891 mL	0.10503 mL	0.05000 mL	3.001	-0.00273	0.39758	0.00021	10.0 s
28:45.1	Data point 28	1.50000 mL	0.10891 mL	0.10757 mL	0.05000 mL	3.191	-0.00242	0.40166	0.00019	10.5 s
29:21.2	Data point 29	1.50000 mL	0.10891 mL	0.10976 mL	0.05000 mL	3.415	-0.00337	0.31261	0.00030	10.0 s
29:56.7	Data point 30	1.50000 mL	0.10891 mL	0.11171 mL	0.05000 mL	3.709	-0.00838	0.53036	0.00057	10.0 s
30:37.3	Data point 31	1.50000 mL	0.10891 mL	0.11310 mL	0.05000 mL	4.012	-0.01267	0.50941	0.00088	11.5 s
31:19.4	Data point 32	1.50000 mL	0.10891 mL	0.11402 mL	0.05000 mL	4.293	-0.01573	0.65616	0.00096	27.0 s
32:11.9	Data point 33	1.50000 mL	0.10891 mL	0.11446 mL	0.05000 mL	4.584	-0.01886	0.90646	0.00098	25.0 s
33:02.3	Data point 34	1.50000 mL	0.10891 mL	0.11475 mL	0.05000 mL	4.896	-0.01935	0.95587	0.00098	18.5 s

Sample name: **M12_octanol**   Experiment start time: **3/1/2018 3:28:52 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01012**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
33:51.3	Data point 35	1.50000 mL	0.10891 mL	0.11491 mL	0.05000 mL	5.148	-0.01470	0.60540	0.00093	26.5 s
34:48.4	Data point 36	1.50000 mL	0.10891 mL	0.11508 mL	0.05000 mL	5.764	-0.01973	0.94931	0.00100	30.0 s
35:49.0	Data point 37	1.50000 mL	0.10891 mL	0.11515 mL	0.05000 mL	6.314	-0.01346	0.55470	0.00089	46.0 s
37:05.6	Data point 38	1.50000 mL	0.10891 mL	0.11524 mL	0.05000 mL	6.936	-0.04576	0.98945	0.00227	Timed out at 59.5 s
38:36.1	Data point 39	1.50000 mL	0.10891 mL	0.11533 mL	0.05000 mL	7.403	-0.05091	0.98174	0.00254	Timed out at 59.5 s
40:11.7	Data point 40	1.50000 mL	0.10891 mL	0.11540 mL	0.05000 mL	7.887	-0.07516	0.99257	0.00373	Timed out at 59.5 s
41:47.3	Data point 41	1.50000 mL	0.10891 mL	0.11547 mL	0.05000 mL	8.267	-0.03226	0.96652	0.00162	Timed out at 59.5 s
43:22.8	Data point 42	1.50000 mL	0.10891 mL	0.11555 mL	0.05000 mL	8.561	-0.01882	0.90027	0.00098	41.0 s
44:39.5	Data point 43	1.50000 mL	0.10891 mL	0.11562 mL	0.05000 mL	8.761	-0.02011	0.98771	0.00100	33.5 s
45:48.7	Data point 44	1.50000 mL	0.10891 mL	0.11571 mL	0.05000 mL	8.967	-0.01575	0.73120	0.00091	19.5 s
46:38.8	Data point 45	1.50000 mL	0.10891 mL	0.11578 mL	0.05000 mL	9.045	-0.01982	0.97953	0.00099	17.0 s
47:53.5	Data point 46	1.50000 mL	0.16860 mL	0.11578 mL	0.25000 mL	1.956	-0.00773	0.91840	0.00040	10.5 s
48:40.3	Data point 47	1.50000 mL	0.16860 mL	0.13525 mL	0.25000 mL	2.168	0.00144	0.01980	0.00051	10.0 s
49:16.0	Data point 48	1.50000 mL	0.16860 mL	0.14760 mL	0.25000 mL	2.388	0.01561	0.79013	0.00087	10.0 s
49:51.7	Data point 49	1.50000 mL	0.16860 mL	0.15534 mL	0.25000 mL	2.573	-0.01149	0.57763	0.00075	10.0 s
50:27.2	Data point 50	1.50000 mL	0.16860 mL	0.16075 mL	0.25000 mL	2.774	0.00396	0.06451	0.00077	10.0 s
51:02.7	Data point 51	1.50000 mL	0.16860 mL	0.16458 mL	0.25000 mL	2.979	-0.00515	0.16315	0.00063	10.0 s
51:38.2	Data point 52	1.50000 mL	0.16860 mL	0.16755 mL	0.25000 mL	3.270	0.00396	0.26107	0.00038	10.0 s
52:18.8	Data point 53	1.50000 mL	0.16860 mL	0.16943 mL	0.25000 mL	3.558	0.01629	0.64793	0.00100	15.5 s
53:05.0	Data point 54	1.50000 mL	0.16860 mL	0.17079 mL	0.25000 mL	3.882	0.01336	0.49641	0.00094	10.5 s
53:46.1	Data point 55	1.50000 mL	0.16860 mL	0.17150 mL	0.25000 mL	4.230	-0.01083	0.45645	0.00079	10.5 s
54:22.0	Data point 56	1.50000 mL	0.16860 mL	0.17187 mL	0.25000 mL	4.682	-0.00156	0.00649	0.00095	13.0 s
55:00.4	Data point 57	1.50000 mL	0.16860 mL	0.17204 mL	0.25000 mL	4.849	-0.00797	0.20959	0.00086	13.0 s
55:43.9	Data point 58	1.50000 mL	0.16860 mL	0.17220 mL	0.25000 mL	5.072	-0.00963	0.30906	0.00086	14.5 s
56:23.8	Data point 59	1.50000 mL	0.16860 mL	0.17227 mL	0.25000 mL	5.214	0.01328	0.44826	0.00098	17.5 s
57:11.9	Data point 60	1.50000 mL	0.16860 mL	0.17239 mL	0.25000 mL	5.360	-0.00926	0.25608	0.00090	13.5 s
58:01.0	Data point 61	1.50000 mL	0.16860 mL	0.17248 mL	0.25000 mL	5.579	0.01451	0.60856	0.00092	24.0 s
58:55.6	Data point 62	1.50000 mL	0.16860 mL	0.17260 mL	0.25000 mL	6.137	-0.01945	0.97898	0.00097	55.5 s
1:00:21.7	Data point 63	1.50000 mL	0.16860 mL	0.17269 mL	0.25000 mL	6.206	0.00784	0.16179	0.00096	13.5 s
1:01:05.7	Data point 64	1.50000 mL	0.16860 mL	0.17277 mL	0.25000 mL	6.406	-0.02142	0.96918	0.00107	Timed out at 59.5 s
1:02:36.2	Data point 65	1.50000 mL	0.16860 mL	0.17281 mL	0.25000 mL	6.193	0.00801	0.28675	0.00074	10.0 s
1:03:11.6	Data point 66	1.50000 mL	0.16860 mL	0.17286 mL	0.25000 mL	6.057	0.00973	0.24043	0.00098	35.0 s
1:04:12.0	Data point 67	1.50000 mL	0.16860 mL	0.17288 mL	0.25000 mL	5.908	0.01936	0.92962	0.00099	39.0 s
1:05:21.4	Data point 68	1.50000 mL	0.16860 mL	0.17293 mL	0.25000 mL	5.918	0.01461	0.56025	0.00096	37.0 s
1:06:23.9	Data point 69	1.50000 mL	0.16860 mL	0.17300 mL	0.25000 mL	5.972	-0.01320	0.59468	0.00085	13.0 s
1:07:07.4	Data point 70	1.50000 mL	0.16860 mL	0.17305 mL	0.25000 mL	6.123	-0.01667	0.70517	0.00098	17.5 s
1:07:55.5	Data point 71	1.50000 mL	0.16860 mL	0.17310 mL	0.25000 mL	6.190	0.01867	0.87098	0.00099	30.5 s
1:08:51.4	Data point 72	1.50000 mL	0.16860 mL	0.17314 mL	0.25000 mL	6.303	-0.00843	0.60418	0.00054	16.0 s
1:09:38.0	Data point 73	1.50000 mL	0.16860 mL	0.17319 mL	0.25000 mL	6.363	-0.01074	0.33367	0.00092	17.0 s
1:10:20.4	Data point 74	1.50000 mL	0.16860 mL	0.17324 mL	0.25000 mL	6.444	-0.01718	0.73214	0.00099	15.0 s
1:11:00.8	Data point 75	1.50000 mL	0.16860 mL	0.17328 mL	0.25000 mL	6.273	0.01956	0.96509	0.00098	57.5 s
1:12:28.9	Data point 76	1.50000 mL	0.16860 mL	0.17345 mL	0.25000 mL	6.967	-0.09221	0.98961	0.00458	Timed out at 59.5 s
1:13:59.4	Data point 77	1.50000 mL	0.16860 mL	0.17359 mL	0.25000 mL	7.698	-0.10796	0.99667	0.00535	Timed out at 59.5 s
1:15:35.0	Data point 78	1.50000 mL	0.16860 mL	0.17366 mL	0.25000 mL	7.761	-0.05693	0.98901	0.00283	Timed out at 59.5 s
1:17:05.5	Data point 79	1.50000 mL	0.16860 mL	0.17373 mL	0.25000 mL	7.873	-0.04996	0.97617	0.00250	Timed out at 59.5 s
1:18:41.2	Data point 80	1.50000 mL	0.16860 mL	0.17380 mL	0.25000 mL	8.062	-0.05264	0.96602	0.00265	Timed out at 59.5 s

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:20:11.7	Data point 81	1.50000 mL	0.16860 mL	0.17385 mL	0.25000 mL	8.128	-0.04768	0.99488	0.00236	Timed out at 59.5 s
1:21:47.4	Data point 82	1.50000 mL	0.16860 mL	0.17392 mL	0.25000 mL	8.346	-0.02426	0.96191	0.00122	Timed out at 59.5 s
1:23:28.3	Data point 83	1.50000 mL	0.16860 mL	0.17401 mL	0.25000 mL	8.532	-0.01603	0.65257	0.00098	28.0 s
1:24:32.0	Data point 84	1.50000 mL	0.16860 mL	0.17411 mL	0.25000 mL	8.645	-0.01972	0.96650	0.00099	46.0 s
1:25:53.8	Data point 85	1.50000 mL	0.16860 mL	0.17418 mL	0.25000 mL	8.779	-0.01801	0.80706	0.00099	22.0 s
1:26:56.6	Data point 86	1.50000 mL	0.16860 mL	0.17429 mL	0.25000 mL	8.994	-0.01105	0.30301	0.00099	14.5 s
1:27:36.5	Data point 87	1.50000 mL	0.16860 mL	0.17432 mL	0.25000 mL	8.985	-0.01268	0.48445	0.00090	22.5 s
1:28:08.1	Assay volumes	1.50000 mL	0.16860 mL	0.17432 mL	0.25000 mL					

Sample name: **M12_octanol** Experiment start time: **3/1/2018 3:28:52 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-01012** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	10%			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.030 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			
Titration 3				

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	3/1/2018 3:28:52 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	3/1/2018 3:28:52 PM	C:\Sirius_T3\HCl18B27.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM
Syringe volume	0.5 mL		

Sample name: **M12_octanol**

Assay name: **pH-metric high logP**

Assay ID: **18C-01012**

Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**

Analyst: **Pion**

Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+2.90 mV		3/1/2018 3:29:20 PM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/28/2018 10:23:32 AM
Wash 2	0.5% Trition X-100 in H20		2/28/2018 10:23:34 AM
Buffer position 1	pH7 Wash		2/28/2018 10:24:06 AM
Buffer position 2	pH 7		2/28/2018 10:24:08 AM
Storage position			2/28/2018 10:21:14 AM
Wash water	8.1e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	7.4e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	112:08:55		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:38] Air gap created for Water (0.15 M KCl)
[2:38] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:39] Air gap released for Water (0.15 M KCl)
[2:44] Titrator arm moved to Titration position
[2:44] Argon flow rate set to 100
[2:44] Titration 1 of 3
[2:44] Adding initial titrants
[2:44] Automatically add 1.50000 mL of water
[3:09] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:09] Stirrer speed set to 10
[3:14] Automatically add 0.02000 mL of Octanol
[3:15] Dispensed 0.019991 mL of Octanol
[3:16] Initial pH = 4.96
[3:16] Iterative adjust 4.96 -> 2.00
[3:16] pH 4.96 -> 2.00
[3:18] Air gap released for Acid (0.5 M HCl)
[3:18] Dispensed 0.052211 mL of Acid (0.5 M HCl)
[3:23] Holding pH 2.00
[5:23] Stirrer speed set to 0
[5:23] Stirrer speed set to 50
[5:23] Iterative adjust 1.89 -> 2.00
[5:23] pH 1.89 -> 2.00
[5:24] Air gap released for Base (0.5 M KOH)
[5:25] Dispensed 0.013288 mL of Base (0.5 M KOH)
[6:15] Stirrer speed set to 0
[6:26] Datapoint id 1 collected
[6:26] Stirrer speed set to 50
[6:31] pH 2.04 -> 2.24
[6:31] Using cautious pH adjust
[6:31] Dispensed 0.007314 mL of Base (0.5 M KOH)
[6:36] Stepping pH = 2.12
[6:36] Dispensed 0.005974 mL of Base (0.5 M KOH)
[6:41] Stepping pH = 2.22
[6:42] Dispensed 0.001105 mL of Base (0.5 M KOH)
[6:47] Stepping pH = 2.24
[7:02] Stirrer speed set to 0
[7:12] Datapoint id 2 collected
[7:12] Charge balance equation is out by 1.6%
[7:12] Stirrer speed set to 50
[7:17] pH 2.26 -> 2.46
[7:17] Using charge balance adjust
[7:17] Dispensed 0.008843 mL of Base (0.5 M KOH)

Sample name: **M12_octanol**　　　　　　　　　　　　Experiment start time: **3/1/2018 3:28:52 PM**
Assay name: **pH-metric high logP**　　　　　　　　　Analyst: **Pion**
Assay ID: **18C-01012**　　　　　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[7:37] Stirrer speed set to 0
[7:47] Datapoint id 3 collected
[7:47] Charge balance equation is out by 4.9%
[7:47] Stirrer speed set to 50
[7:53] pH 2.48 -> 2.68
[7:53] Using charge balance adjust
[7:53] Dispensed 0.005456 mL of Base (0.5 M KOH)
[8:13] Stirrer speed set to 0
[8:41] Datapoint id 4 collected
[8:41] Charge balance equation is out by -2.2%
[8:41] Stirrer speed set to 50
[8:46] pH 2.68 -> 2.88
[8:46] Using charge balance adjust
[8:46] Dispensed 0.003622 mL of Base (0.5 M KOH)
[9:07] Stirrer speed set to 0
[9:17] Datapoint id 5 collected
[9:17] Charge balance equation is out by 9.1%
[9:17] Stirrer speed set to 50
[9:22] pH 2.90 -> 3.10
[9:22] Using charge balance adjust
[9:22] Dispensed 0.002493 mL of Base (0.5 M KOH)
[9:42] Stirrer speed set to 0
[9:52] Datapoint id 6 collected
[9:52] Charge balance equation is out by -16.5%
[9:52] Stirrer speed set to 50
[9:57] pH 3.07 -> 3.27
[9:57] Using cautious pH adjust
[9:57] Dispensed 0.001011 mL of Base (0.5 M KOH)
[10:02] Stepping pH = 3.12
[10:02] Dispensed 0.001317 mL of Base (0.5 M KOH)
[10:08] Stepping pH = 3.24
[10:08] Dispensed 0.000212 mL of Base (0.5 M KOH)
[10:13] Stepping pH = 3.25
[10:13] Dispensed 0.000212 mL of Base (0.5 M KOH)
[10:18] Stepping pH = 3.27
[10:33] Stirrer speed set to 0
[10:44] Datapoint id 7 collected
[10:44] Charge balance equation is out by -36.5%
[10:44] Stirrer speed set to 50
[10:49] pH 3.27 -> 3.47
[10:49] Using cautious pH adjust
[10:49] Dispensed 0.000894 mL of Base (0.5 M KOH)
[10:54] Stepping pH = 3.35
[10:54] Dispensed 0.000847 mL of Base (0.5 M KOH)
[10:59] Stepping pH = 3.46
[11:14] Stirrer speed set to 0
[11:25] Datapoint id 8 collected
[11:25] Charge balance equation is out by 2.1%
[11:25] Stirrer speed set to 50
[11:30] pH 3.48 -> 3.68
[11:30] Using charge balance adjust
[11:30] Dispensed 0.001693 mL of Base (0.5 M KOH)
[11:50] Stirrer speed set to 0
[12:01] Datapoint id 9 collected
[12:01] Charge balance equation is out by 39.1%
[12:01] Stirrer speed set to 50
[12:06] pH 3.73 -> 3.93
[12:06] Using cautious pH adjust
[12:06] Dispensed 0.000823 mL of Base (0.5 M KOH)

Sample name: **M12_octanol**

Assay name: **pH-metric high logP**

Assay ID: **18C-01012**

Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**

Analyst: **Pion**

Instrument ID: **T312060**

Experiment Log (continued)

[12:11] Stepping pH = 3.85
[12:11] Dispensed 0.000447 mL of Base (0.5 M KOH)
[12:16] Stepping pH = 3.94
[12:31] Stirrer speed set to 0
[12:45] Datapoint id 10 collected
[12:45] Charge balance equation is out by 22.7%
[12:45] Stirrer speed set to 50
[12:50] pH 3.90 -> 4.10
[12:50] Using cautious pH adjust
[12:51] Dispensed 0.000800 mL of Base (0.5 M KOH)
[12:56] Stepping pH = 4.04
[12:56] Dispensed 0.000306 mL of Base (0.5 M KOH)
[13:01] Stepping pH = 4.12
[13:16] Stirrer speed set to 0
[13:29] Datapoint id 11 collected
[13:29] Charge balance equation is out by 30.8%
[13:29] Stirrer speed set to 50
[13:34] pH 4.13 -> 4.33
[13:34] Using cautious pH adjust
[13:34] Dispensed 0.000706 mL of Base (0.5 M KOH)
[13:39] Stepping pH = 4.30
[13:39] Dispensed 0.000094 mL of Base (0.5 M KOH)
[13:44] Stepping pH = 4.35
[14:00] Stirrer speed set to 0
[14:14] Datapoint id 12 collected
[14:14] Charge balance equation is out by 42.4%
[14:14] Stirrer speed set to 50
[14:19] pH 4.31 -> 4.51
[14:19] Using cautious pH adjust
[14:19] Dispensed 0.000588 mL of Base (0.5 M KOH)
[14:24] Stepping pH = 4.55
[14:39] Stirrer speed set to 0
[14:56] Datapoint id 13 collected
[14:56] Charge balance equation is out by 50.0%
[14:56] Stirrer speed set to 50
[15:01] pH 4.55 -> 4.75
[15:01] Using cautious pH adjust
[15:01] Dispensed 0.000423 mL of Base (0.5 M KOH)
[15:06] Stepping pH = 4.83
[15:21] Stirrer speed set to 0
[15:44] Datapoint id 14 collected
[15:44] Charge balance equation is out by 50.0%
[15:44] Stirrer speed set to 50
[15:50] pH 4.82 -> 5.02
[15:50] Using cautious pH adjust
[15:50] Dispensed 0.000259 mL of Base (0.5 M KOH)
[15:55] Stepping pH = 4.97
[15:55] Dispensed 0.000071 mL of Base (0.5 M KOH)
[16:00] Stepping pH = 5.06
[16:15] Stirrer speed set to 0
[16:43] Datapoint id 15 collected
[16:43] Charge balance equation is out by 38.3%
[16:43] Stirrer speed set to 50
[16:48] pH 5.02 -> 5.22
[16:48] Using cautious pH adjust
[16:48] Dispensed 0.000188 mL of Base (0.5 M KOH)
[16:53] Stepping pH = 5.44
[17:08] Stirrer speed set to 0
[17:38] Datapoint id 16 collected

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[17:38] Charge balance equation is out by 50.0%
[17:38] Stirrer speed set to 50
[17:43] pH 5.43 -> 5.63
[17:43] Using cautious pH adjust
[17:43] Dispensed 0.000094 mL of Base (0.5 M KOH)
[17:48] Stepping pH = 5.54
[17:48] Dispensed 0.000047 mL of Base (0.5 M KOH)
[17:53] Stepping pH = 5.77
[18:08] Stirrer speed set to 0
[18:40] Datapoint id 17 collected
[18:40] Charge balance equation is out by 18.4%
[18:40] Stirrer speed set to 50
[18:45] pH 5.84 -> 6.04
[18:45] Using cautious pH adjust
[18:45] Dispensed 0.000047 mL of Base (0.5 M KOH)
[18:50] Stepping pH = 5.88
[18:50] Dispensed 0.000094 mL of Base (0.5 M KOH)
[18:55] Stepping pH = 6.68
[19:11] Stirrer speed set to 0
[20:11] Datapoint id 18 collected
[20:11] Charge balance equation is out by -44.4%
[20:11] Stirrer speed set to 50
[20:16] pH 6.88 -> 7.08
[20:16] Using cautious pH adjust
[20:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[20:21] Stepping pH = 6.87
[20:21] Dispensed 0.000071 mL of Base (0.5 M KOH)
[20:26] Stepping pH = 7.48
[20:41] Stirrer speed set to 0
[21:41] Datapoint id 19 collected
[21:41] Charge balance equation is out by -232.0%
[21:41] Stirrer speed set to 50
[21:46] pH 7.52 -> 7.72
[21:46] Using cautious pH adjust
[21:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[21:51] Stepping pH = 7.42
[21:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[21:56] Stepping pH = 7.45
[21:57] Dispensed 0.000094 mL of Base (0.5 M KOH)
[22:02] Stepping pH = 8.76
[22:17] Stirrer speed set to 0
[23:10] Datapoint id 20 collected
[23:10] Charge balance equation is out by -1,588.8%
[23:10] Stirrer speed set to 50
[23:15] pH 8.90 -> 9.05
[23:15] Using cautious pH adjust
[23:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[23:21] Stepping pH = 8.90
[23:21] Dispensed 0.000071 mL of Base (0.5 M KOH)
[23:26] Stepping pH = 9.05
[23:41] Stirrer speed set to 0
[24:07] Datapoint id 21 collected
[24:07] Charge balance equation is out by -237.3%
[24:07] Titration 2 of 3
[24:07] Adding initial titrants
[24:07] Automatically add 0.03000 mL of Octanol
[24:08] Dispensed 0.030009 mL of Octanol
[24:08] Stirrer speed set to 10
[24:09] Stirrer speed set to 55

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[24:09] Iterative adjust 9.11 -> 2.00
[24:09] pH 9.11 -> 2.00
[24:10] Dispensed 0.056703 mL of Acid (0.5 M HCl)
[25:01] Stirrer speed set to 0
[25:11] Datapoint id 22 collected
[25:11] Stirrer speed set to 55
[25:16] pH 1.96 -> 2.16
[25:16] Using cautious pH adjust
[25:16] Dispensed 0.009572 mL of Base (0.5 M KOH)
[25:22] Stepping pH = 2.04
[25:22] Dispensed 0.007832 mL of Base (0.5 M KOH)
[25:27] Stepping pH = 2.13
[25:27] Dispensed 0.001458 mL of Base (0.5 M KOH)
[25:32] Stepping pH = 2.16
[25:47] Stirrer speed set to 0
[25:57] Datapoint id 23 collected
[25:57] Charge balance equation is out by 1.5%
[25:57] Stirrer speed set to 55
[26:02] pH 2.17 -> 2.37
[26:02] Using charge balance adjust
[26:03] Dispensed 0.011618 mL of Base (0.5 M KOH)
[26:23] Stirrer speed set to 0
[26:33] Datapoint id 24 collected
[26:33] Charge balance equation is out by 8.1%
[26:33] Stirrer speed set to 55
[26:38] pH 2.40 -> 2.60
[26:38] Using charge balance adjust
[26:38] Dispensed 0.007079 mL of Base (0.5 M KOH)
[26:58] Stirrer speed set to 0
[27:09] Datapoint id 25 collected
[27:09] Charge balance equation is out by -3.0%
[27:09] Stirrer speed set to 55
[27:14] pH 2.60 -> 2.80
[27:14] Using charge balance adjust
[27:14] Dispensed 0.004704 mL of Base (0.5 M KOH)
[27:35] Stirrer speed set to 0
[27:45] Datapoint id 26 collected
[27:45] Charge balance equation is out by 9.3%
[27:45] Stirrer speed set to 55
[27:50] pH 2.82 -> 3.02
[27:50] Using charge balance adjust
[27:50] Dispensed 0.003175 mL of Base (0.5 M KOH)
[28:10] Stirrer speed set to 0
[28:20] Datapoint id 27 collected
[28:20] Charge balance equation is out by -11.4%
[28:20] Stirrer speed set to 55
[28:25] pH 3.00 -> 3.20
[28:25] Using charge balance adjust
[28:25] Dispensed 0.002540 mL of Base (0.5 M KOH)
[28:46] Stirrer speed set to 0
[28:56] Datapoint id 28 collected
[28:56] Charge balance equation is out by -6.4%
[28:56] Stirrer speed set to 55
[29:01] pH 3.19 -> 3.39
[29:01] Using charge balance adjust
[29:01] Dispensed 0.002187 mL of Base (0.5 M KOH)
[29:22] Stirrer speed set to 0
[29:32] Datapoint id 29 collected
[29:32] Charge balance equation is out by 13.7%

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[29:32] Stirrer speed set to 55
[29:37] pH 3.42 -> 3.62
[29:37] Using charge balance adjust
[29:37] Dispensed 0.001952 mL of Base (0.5 M KOH)
[29:57] Stirrer speed set to 0
[30:07] Datapoint id 30 collected
[30:07] Charge balance equation is out by 46.6%
[30:07] Stirrer speed set to 55
[30:12] pH 3.71 -> 3.91
[30:12] Using cautious pH adjust
[30:12] Dispensed 0.000870 mL of Base (0.5 M KOH)
[30:17] Stepping pH = 3.82
[30:18] Dispensed 0.000517 mL of Base (0.5 M KOH)
[30:23] Stepping pH = 3.94
[30:38] Stirrer speed set to 0
[30:49] Datapoint id 31 collected
[30:49] Charge balance equation is out by 20.1%
[30:49] Stirrer speed set to 55
[30:54] pH 4.01 -> 4.21
[30:54] Using cautious pH adjust
[30:55] Dispensed 0.000659 mL of Base (0.5 M KOH)
[31:00] Stepping pH = 4.14
[31:00] Dispensed 0.000259 mL of Base (0.5 M KOH)
[31:05] Stepping pH = 4.27
[31:20] Stirrer speed set to 0
[31:47] Datapoint id 32 collected
[31:47] Charge balance equation is out by 30.0%
[31:47] Stirrer speed set to 55
[31:52] pH 4.31 -> 4.51
[31:52] Using cautious pH adjust
[31:52] Dispensed 0.000447 mL of Base (0.5 M KOH)
[31:57] Stepping pH = 4.55
[32:12] Stirrer speed set to 0
[32:37] Datapoint id 33 collected
[32:37] Charge balance equation is out by 50.0%
[32:37] Stirrer speed set to 55
[32:42] pH 4.60 -> 4.80
[32:42] Using cautious pH adjust
[32:43] Dispensed 0.000282 mL of Base (0.5 M KOH)
[32:48] Stepping pH = 4.90
[33:03] Stirrer speed set to 0
[33:21] Datapoint id 34 collected
[33:21] Charge balance equation is out by 50.0%
[33:21] Stirrer speed set to 55
[33:26] pH 4.92 -> 5.12
[33:26] Using cautious pH adjust
[33:26] Dispensed 0.000141 mL of Base (0.5 M KOH)
[33:32] Stepping pH = 5.08
[33:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[33:37] Stepping pH = 5.15
[33:52] Stirrer speed set to 0
[34:18] Datapoint id 35 collected
[34:18] Charge balance equation is out by 40.7%
[34:18] Stirrer speed set to 55
[34:23] pH 5.16 -> 5.36
[34:23] Using cautious pH adjust
[34:23] Dispensed 0.000094 mL of Base (0.5 M KOH)
[34:29] Stepping pH = 5.26
[34:29] Dispensed 0.000071 mL of Base (0.5 M KOH)

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[34:34] Stepping pH = 5.69
[34:49] Stirrer speed set to 0
[35:19] Datapoint id 36 collected
[35:19] Charge balance equation is out by 17.2%
[35:19] Stirrer speed set to 55
[35:24] pH 5.79 -> 5.99
[35:24] Using cautious pH adjust
[35:24] Dispensed 0.000047 mL of Base (0.5 M KOH)
[35:29] Stepping pH = 5.93
[35:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[35:34] Stepping pH = 6.19
[35:49] Stirrer speed set to 0
[36:36] Datapoint id 37 collected
[36:36] Charge balance equation is out by 23.2%
[36:36] Stirrer speed set to 55
[36:41] pH 6.24 -> 6.44
[36:41] Using cautious pH adjust
[36:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:46] Stepping pH = 6.26
[36:46] Dispensed 0.000071 mL of Base (0.5 M KOH)
[36:51] Stepping pH = 6.71
[37:06] Stirrer speed set to 0
[38:06] Datapoint id 38 collected
[38:06] Charge balance equation is out by -67.6%
[38:06] Stirrer speed set to 55
[38:11] pH 6.80 -> 7.00
[38:11] Using cautious pH adjust
[38:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:16] Stepping pH = 6.78
[38:16] Dispensed 0.000071 mL of Base (0.5 M KOH)
[38:21] Stepping pH = 7.04
[38:37] Stirrer speed set to 0
[39:37] Datapoint id 39 collected
[39:37] Charge balance equation is out by -246.2%
[39:37] Stirrer speed set to 55
[39:42] pH 7.29 -> 7.49
[39:42] Using cautious pH adjust
[39:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:47] Stepping pH = 7.29
[39:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:52] Stepping pH = 7.41
[39:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:57] Stepping pH = 7.70
[40:12] Stirrer speed set to 0
[41:12] Datapoint id 40 collected
[41:12] Charge balance equation is out by -384.4%
[41:12] Stirrer speed set to 55
[41:17] pH 7.79 -> 7.99
[41:17] Using cautious pH adjust
[41:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:22] Stepping pH = 7.81
[41:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:28] Stepping pH = 7.95
[41:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:33] Stepping pH = 8.17
[41:48] Stirrer speed set to 0
[42:48] Datapoint id 41 collected
[42:48] Charge balance equation is out by -765.5%
[42:48] Stirrer speed set to 55

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[42:53] pH 8.18 -> 8.38
[42:53] Using cautious pH adjust
[42:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:58] Stepping pH = 8.17
[42:58] Dispensed 0.000024 mL of Base (0.5 M KOH)
[43:03] Stepping pH = 8.32
[43:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[43:08] Stepping pH = 8.51
[43:23] Stirrer speed set to 0
[44:04] Datapoint id 42 collected
[44:04] Charge balance equation is out by -611.1%
[44:04] Stirrer speed set to 55
[44:09] pH 8.54 -> 8.74
[44:09] Using cautious pH adjust
[44:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[44:15] Stepping pH = 8.56
[44:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[44:20] Stepping pH = 8.64
[44:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[44:25] Stepping pH = 8.75
[44:40] Stirrer speed set to 0
[45:14] Datapoint id 43 collected
[45:14] Charge balance equation is out by -275.0%
[45:14] Stirrer speed set to 55
[45:19] pH 8.74 -> 8.94
[45:19] Using cautious pH adjust
[45:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[45:24] Stepping pH = 8.74
[45:24] Dispensed 0.000047 mL of Base (0.5 M KOH)
[45:29] Stepping pH = 8.86
[45:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[45:34] Stepping pH = 8.97
[45:49] Stirrer speed set to 0
[46:09] Datapoint id 44 collected
[46:09] Charge balance equation is out by -212.1%
[46:09] Stirrer speed set to 55
[46:14] pH 8.94 -> 9.05
[46:14] Using cautious pH adjust
[46:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[46:19] Stepping pH = 8.94
[46:19] Dispensed 0.000047 mL of Base (0.5 M KOH)
[46:24] Stepping pH = 9.01
[46:39] Stirrer speed set to 0
[46:56] Datapoint id 45 collected
[46:56] Charge balance equation is out by -261.0%
[46:56] Titration 3 of 3
[46:56] Adding initial titrants
[46:56] Automatically add 0.20000 mL of Octanol
[47:01] Dispensed 0.200000 mL of Octanol
[47:01] Stirrer speed set to 10
[47:02] Stirrer speed set to 60
[47:02] Iterative adjust 9.05 -> 2.00
[47:02] pH 9.05 -> 2.00
[47:04] Dispensed 0.059690 mL of Acid (0.5 M HCl)
[47:54] Stirrer speed set to 0
[48:04] Datapoint id 46 collected
[48:04] Stirrer speed set to 60
[48:10] pH 1.96 -> 2.16
[48:10] Using cautious pH adjust

Sample name: **M12_octanol** Experiment start time: **3/1/2018 3:28:52 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-01012** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[48:10] Dispensed 0.010113 mL of Base (0.5 M KOH)
[48:15] Stepping pH = 2.05
[48:15] Dispensed 0.007361 mL of Base (0.5 M KOH)
[48:20] Stepping pH = 2.13
[48:21] Dispensed 0.001999 mL of Base (0.5 M KOH)
[48:26] Stepping pH = 2.16
[48:41] Stirrer speed set to 0
[48:51] Datapoint id 47 collected
[48:51] Charge balance equation is out by 3.8%
[48:51] Stirrer speed set to 60
[48:56] pH 2.18 -> 2.38
[48:56] Using charge balance adjust
[48:56] Dispensed 0.012347 mL of Base (0.5 M KOH)
[49:16] Stirrer speed set to 0
[49:27] Datapoint id 48 collected
[49:27] Charge balance equation is out by 4.8%
[49:27] Stirrer speed set to 60
[49:32] pH 2.39 -> 2.59
[49:32] Using charge balance adjust
[49:32] Dispensed 0.007738 mL of Base (0.5 M KOH)
[49:52] Stirrer speed set to 0
[50:02] Datapoint id 49 collected
[50:02] Charge balance equation is out by -10.9%
[50:02] Stirrer speed set to 60
[50:07] pH 2.58 -> 2.78
[50:07] Using charge balance adjust
[50:07] Dispensed 0.005409 mL of Base (0.5 M KOH)
[50:28] Stirrer speed set to 0
[50:38] Datapoint id 50 collected
[50:38] Charge balance equation is out by -1.8%
[50:38] Stirrer speed set to 60
[50:43] pH 2.78 -> 2.98
[50:43] Using charge balance adjust
[50:43] Dispensed 0.003833 mL of Base (0.5 M KOH)
[51:03] Stirrer speed set to 0
[51:13] Datapoint id 51 collected
[51:13] Charge balance equation is out by -0.7%
[51:13] Stirrer speed set to 60
[51:18] pH 2.99 -> 3.19
[51:18] Using charge balance adjust
[51:18] Dispensed 0.002963 mL of Base (0.5 M KOH)
[51:39] Stirrer speed set to 0
[51:49] Datapoint id 52 collected
[51:49] Charge balance equation is out by 41.2%
[51:49] Stirrer speed set to 60
[51:54] pH 3.28 -> 3.48
[51:54] Using cautious pH adjust
[51:54] Dispensed 0.001152 mL of Base (0.5 M KOH)
[51:59] Stepping pH = 3.38
[51:59] Dispensed 0.000729 mL of Base (0.5 M KOH)
[52:04] Stepping pH = 3.51
[52:19] Stirrer speed set to 0
[52:35] Datapoint id 53 collected
[52:35] Charge balance equation is out by 18.3%
[52:35] Stirrer speed set to 60
[52:40] pH 3.56 -> 3.76
[52:40] Using cautious pH adjust
[52:40] Dispensed 0.000917 mL of Base (0.5 M KOH)
[52:45] Stepping pH = 3.68

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[52:45] Dispensed 0.000447 mL of Base (0.5 M KOH)
[52:50] Stepping pH = 3.81
[53:05] Stirrer speed set to 0
[53:16] Datapoint id 54 collected
[53:16] Charge balance equation is out by 25.4%
[53:16] Stirrer speed set to 60
[53:21] pH 3.89 -> 4.09
[53:21] Using cautious pH adjust
[53:21] Dispensed 0.000659 mL of Base (0.5 M KOH)
[53:26] Stepping pH = 4.07
[53:26] Dispensed 0.000047 mL of Base (0.5 M KOH)
[53:31] Stepping pH = 4.21
[53:47] Stirrer speed set to 0
[53:57] Datapoint id 55 collected
[53:57] Charge balance equation is out by 45.6%
[53:57] Stirrer speed set to 60
[54:02] pH 4.23 -> 4.43
[54:02] Using cautious pH adjust
[54:02] Dispensed 0.000376 mL of Base (0.5 M KOH)
[54:07] Stepping pH = 4.66
[54:22] Stirrer speed set to 0
[54:35] Datapoint id 56 collected
[54:35] Charge balance equation is out by 50.0%
[54:35] Stirrer speed set to 60
[54:41] pH 4.69 -> 4.89
[54:41] Using cautious pH adjust
[54:41] Dispensed 0.000165 mL of Base (0.5 M KOH)
[54:46] Stepping pH = 4.90
[55:01] Stirrer speed set to 0
[55:14] Datapoint id 57 collected
[55:14] Charge balance equation is out by 50.0%
[55:14] Stirrer speed set to 60
[55:19] pH 4.82 -> 5.02
[55:19] Using cautious pH adjust
[55:19] Dispensed 0.000118 mL of Base (0.5 M KOH)
[55:24] Stepping pH = 4.96
[55:24] Dispensed 0.000047 mL of Base (0.5 M KOH)
[55:29] Stepping pH = 5.07
[55:44] Stirrer speed set to 0
[55:59] Datapoint id 58 collected
[55:59] Charge balance equation is out by 35.4%
[55:59] Stirrer speed set to 60
[56:04] pH 5.04 -> 5.24
[56:04] Using cautious pH adjust
[56:04] Dispensed 0.000071 mL of Base (0.5 M KOH)
[56:09] Stepping pH = 5.24
[56:24] Stirrer speed set to 0
[56:42] Datapoint id 59 collected
[56:42] Charge balance equation is out by 50.0%
[56:42] Stirrer speed set to 60
[56:47] pH 5.18 -> 5.38
[56:47] Using cautious pH adjust
[56:47] Dispensed 0.000071 mL of Base (0.5 M KOH)
[56:52] Stepping pH = 5.28
[56:52] Dispensed 0.000047 mL of Base (0.5 M KOH)
[56:57] Stepping pH = 5.44
[57:12] Stirrer speed set to 0
[57:26] Datapoint id 60 collected
[57:26] Charge balance equation is out by 17.2%

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[57:26] Stirrer speed set to 60
[57:31] pH 5.44 -> 5.64
[57:31] Using cautious pH adjust
[57:31] Dispensed 0.000047 mL of Base (0.5 M KOH)
[57:36] Stepping pH = 5.52
[57:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:41] Stepping pH = 5.57
[57:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:46] Stepping pH = 5.67
[58:01] Stirrer speed set to 0
[58:26] Datapoint id 61 collected
[58:26] Charge balance equation is out by -31.4%
[58:26] Stirrer speed set to 60
[58:31] pH 5.57 -> 5.77
[58:31] Using cautious pH adjust
[58:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:36] Stepping pH = 5.60
[58:36] Dispensed 0.000094 mL of Base (0.5 M KOH)
[58:41] Stepping pH = 6.29
[58:56] Stirrer speed set to 0
[59:52] Datapoint id 62 collected
[59:52] Charge balance equation is out by -71.8%
[59:52] Stirrer speed set to 60
[59:57] pH 5.94 -> 6.14
[59:57] Using cautious pH adjust
[59:57] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:02] Stepping pH = 5.95
[1:00:02] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:00:07] Stepping pH = 6.30
[1:00:22] Stirrer speed set to 0
[1:00:36] Datapoint id 63 collected
[1:00:36] Charge balance equation is out by -89.9%
[1:00:36] Stirrer speed set to 60
[1:00:41] pH 6.12 -> 6.32
[1:00:41] Using cautious pH adjust
[1:00:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:46] Stepping pH = 6.16
[1:00:46] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:00:51] Stepping pH = 6.48
[1:01:06] Stirrer speed set to 0
[1:02:06] Datapoint id 64 collected
[1:02:06] Charge balance equation is out by -38.2%
[1:02:06] Stirrer speed set to 60
[1:02:11] pH 6.11 -> 6.31
[1:02:11] Using cautious pH adjust
[1:02:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:16] Stepping pH = 6.18
[1:02:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:22] Stepping pH = 6.34
[1:02:37] Stirrer speed set to 0
[1:02:47] Datapoint id 65 collected
[1:02:47] Charge balance equation is out by -6.6%
[1:02:47] Stirrer speed set to 60
[1:02:52] pH 6.05 -> 6.25
[1:02:52] Using charge balance adjust
[1:02:52] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:03:12] Stirrer speed set to 0
[1:03:47] Datapoint id 66 collected
[1:03:47] Charge balance equation is out by -98.3%

Experiment Log (continued)

[1:03:47] Stirrer speed set to 60
[1:03:52] pH 5.78 -> 5.98
[1:03:52] Using cautious pH adjust
[1:03:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:57] Stepping pH = 5.98
[1:04:12] Stirrer speed set to 0
[1:04:52] Datapoint id 67 collected
[1:04:52] Charge balance equation is out by 50.0%
[1:04:52] Stirrer speed set to 60
[1:04:57] pH 5.76 -> 5.96
[1:04:57] Using cautious pH adjust
[1:04:57] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:05:02] Stepping pH = 5.85
[1:05:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:05:07] Stepping pH = 6.07
[1:05:22] Stirrer speed set to 0
[1:05:59] Datapoint id 68 collected
[1:05:59] Charge balance equation is out by 7.8%
[1:05:59] Stirrer speed set to 60
[1:06:04] pH 5.71 -> 5.91
[1:06:04] Using charge balance adjust
[1:06:04] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:06:24] Stirrer speed set to 0
[1:06:37] Datapoint id 69 collected
[1:06:37] Charge balance equation is out by 33.1%
[1:06:37] Stirrer speed set to 60
[1:06:42] pH 5.84 -> 6.04
[1:06:42] Using cautious pH adjust
[1:06:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:06:48] Stepping pH = 5.96
[1:06:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:06:53] Stepping pH = 6.21
[1:07:08] Stirrer speed set to 0
[1:07:25] Datapoint id 70 collected
[1:07:25] Charge balance equation is out by 15.2%
[1:07:25] Stirrer speed set to 60
[1:07:30] pH 5.94 -> 6.14
[1:07:30] Using cautious pH adjust
[1:07:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:36] Stepping pH = 6.12
[1:07:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:41] Stepping pH = 6.28
[1:07:56] Stirrer speed set to 0
[1:08:27] Datapoint id 71 collected
[1:08:27] Charge balance equation is out by 14.3%
[1:08:27] Stirrer speed set to 60
[1:08:32] pH 6.04 -> 6.24
[1:08:32] Using charge balance adjust
[1:08:32] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:08:52] Stirrer speed set to 0
[1:09:08] Datapoint id 72 collected
[1:09:08] Charge balance equation is out by 29.3%
[1:09:08] Stirrer speed set to 60
[1:09:13] pH 6.21 -> 6.41
[1:09:13] Using cautious pH adjust
[1:09:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:18] Stepping pH = 6.32
[1:09:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:23] Stepping pH = 6.47

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:09:38] Stirrer speed set to 0
[1:09:55] Datapoint id 73 collected
[1:09:55] Charge balance equation is out by 11.9%
[1:09:55] Stirrer speed set to 60
[1:10:01] pH 6.23 -> 6.43
[1:10:01] Using charge balance adjust
[1:10:01] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:10:21] Stirrer speed set to 0
[1:10:36] Datapoint id 74 collected
[1:10:36] Charge balance equation is out by 6.5%
[1:10:36] Stirrer speed set to 60
[1:10:41] pH 6.39 -> 6.59
[1:10:41] Using charge balance adjust
[1:10:41] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:11:01] Stirrer speed set to 0
[1:11:59] Datapoint id 75 collected
[1:11:59] Charge balance equation is out by -41.6%
[1:11:59] Stirrer speed set to 60
[1:12:04] pH 5.94 -> 6.14
[1:12:04] Using cautious pH adjust
[1:12:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:12:09] Stepping pH = 5.92
[1:12:09] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:12:14] Stepping pH = 7.15
[1:12:29] Stirrer speed set to 0
[1:13:29] Datapoint id 76 collected
[1:13:29] Charge balance equation is out by -219.5%
[1:13:29] Stirrer speed set to 60
[1:13:34] pH 6.70 -> 6.90
[1:13:34] Using cautious pH adjust
[1:13:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:13:40] Stepping pH = 6.66
[1:13:40] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:13:45] Stepping pH = 7.66
[1:14:00] Stirrer speed set to 0
[1:15:00] Datapoint id 77 collected
[1:15:00] Charge balance equation is out by -255.5%
[1:15:00] Stirrer speed set to 60
[1:15:05] pH 7.53 -> 7.73
[1:15:05] Using cautious pH adjust
[1:15:05] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:15:10] Stepping pH = 7.55
[1:15:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:15:15] Stepping pH = 7.66
[1:15:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:15:20] Stepping pH = 7.84
[1:15:35] Stirrer speed set to 0
[1:16:35] Datapoint id 78 collected
[1:16:35] Charge balance equation is out by -467.5%
[1:16:35] Stirrer speed set to 60
[1:16:41] pH 7.53 -> 7.73
[1:16:41] Using cautious pH adjust
[1:16:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:16:46] Stepping pH = 7.43
[1:16:46] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:16:51] Stepping pH = 7.78
[1:17:06] Stirrer speed set to 0
[1:18:06] Datapoint id 79 collected
[1:18:06] Charge balance equation is out by -479.6%

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
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Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:18:06] Stirrer speed set to 60
[1:18:11] pH 7.85 -> 8.05
[1:18:11] Using cautious pH adjust
[1:18:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:18:16] Stepping pH = 7.94
[1:18:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:18:21] Stepping pH = 8.03
[1:18:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:18:27] Stepping pH = 8.07
[1:18:42] Stirrer speed set to 0
[1:19:42] Datapoint id 80 collected
[1:19:42] Charge balance equation is out by -636.5%
[1:19:42] Stirrer speed set to 60
[1:19:47] pH 7.94 -> 8.14
[1:19:47] Using cautious pH adjust
[1:19:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:52] Stepping pH = 8.03
[1:19:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:57] Stepping pH = 8.17
[1:20:12] Stirrer speed set to 0
[1:21:12] Datapoint id 81 collected
[1:21:12] Charge balance equation is out by -388.4%
[1:21:12] Stirrer speed set to 60
[1:21:17] pH 8.07 -> 8.27
[1:21:17] Using cautious pH adjust
[1:21:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:21:22] Stepping pH = 8.13
[1:21:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:21:28] Stepping pH = 8.23
[1:21:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:21:33] Stepping pH = 8.37
[1:21:48] Stirrer speed set to 0
[1:22:48] Datapoint id 82 collected
[1:22:48] Charge balance equation is out by -583.2%
[1:22:48] Stirrer speed set to 60
[1:22:53] pH 8.38 -> 8.58
[1:22:53] Using cautious pH adjust
[1:22:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:22:58] Stepping pH = 8.43
[1:22:58] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:03] Stepping pH = 8.46
[1:23:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:08] Stepping pH = 8.54
[1:23:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:14] Stepping pH = 8.63
[1:23:29] Stirrer speed set to 0
[1:23:57] Datapoint id 83 collected
[1:23:57] Charge balance equation is out by -489.1%
[1:23:57] Stirrer speed set to 60
[1:24:02] pH 8.48 -> 8.68
[1:24:02] Using cautious pH adjust
[1:24:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:24:07] Stepping pH = 8.46
[1:24:07] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:24:12] Stepping pH = 8.59
[1:24:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:24:17] Stepping pH = 8.68
[1:24:32] Stirrer speed set to 0
[1:25:19] Datapoint id 84 collected

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01012_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 3:28:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:25:19] Charge balance equation is out by -472.3%
[1:25:19] Stirrer speed set to 60
[1:25:24] pH 8.61 -> 8.81
[1:25:24] Using cautious pH adjust
[1:25:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:25:29] Stepping pH = 8.65
[1:25:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:25:34] Stepping pH = 8.72
[1:25:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:25:39] Stepping pH = 8.80
[1:25:54] Stirrer speed set to 0
[1:26:16] Datapoint id 85 collected
[1:26:16] Charge balance equation is out by -185.7%
[1:26:16] Stirrer speed set to 60
[1:26:21] pH 8.77 -> 8.97
[1:26:21] Using cautious pH adjust
[1:26:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:27] Stepping pH = 8.79
[1:26:27] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:26:32] Stepping pH = 8.90
[1:26:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:37] Stepping pH = 8.95
[1:26:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:42] Stepping pH = 9.00
[1:26:57] Stirrer speed set to 0
[1:27:12] Datapoint id 86 collected
[1:27:12] Charge balance equation is out by -250.7%
[1:27:12] Stirrer speed set to 60
[1:27:17] pH 8.99 -> 9.05
[1:27:17] Using cautious pH adjust
[1:27:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:27:22] Stepping pH = 9.00
[1:27:37] Stirrer speed set to 0
[1:27:59] Datapoint id 87 collected
[1:27:59] Charge balance equation is out by -76.9%
[1:27:59] Argon flow rate set to 0
[1:28:03] Titrator arm moved over Titration position